CHEMISTRY
A EUROPEAN JOURNAL

Supporting Information

Heptametallic, Octupolar Nonlinear Optical Chromophores with Six Ferrocenyl Substituents

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chem_201204453_sm_miscellaneous_information.pdf

1. Colour Versions of Figures from Article

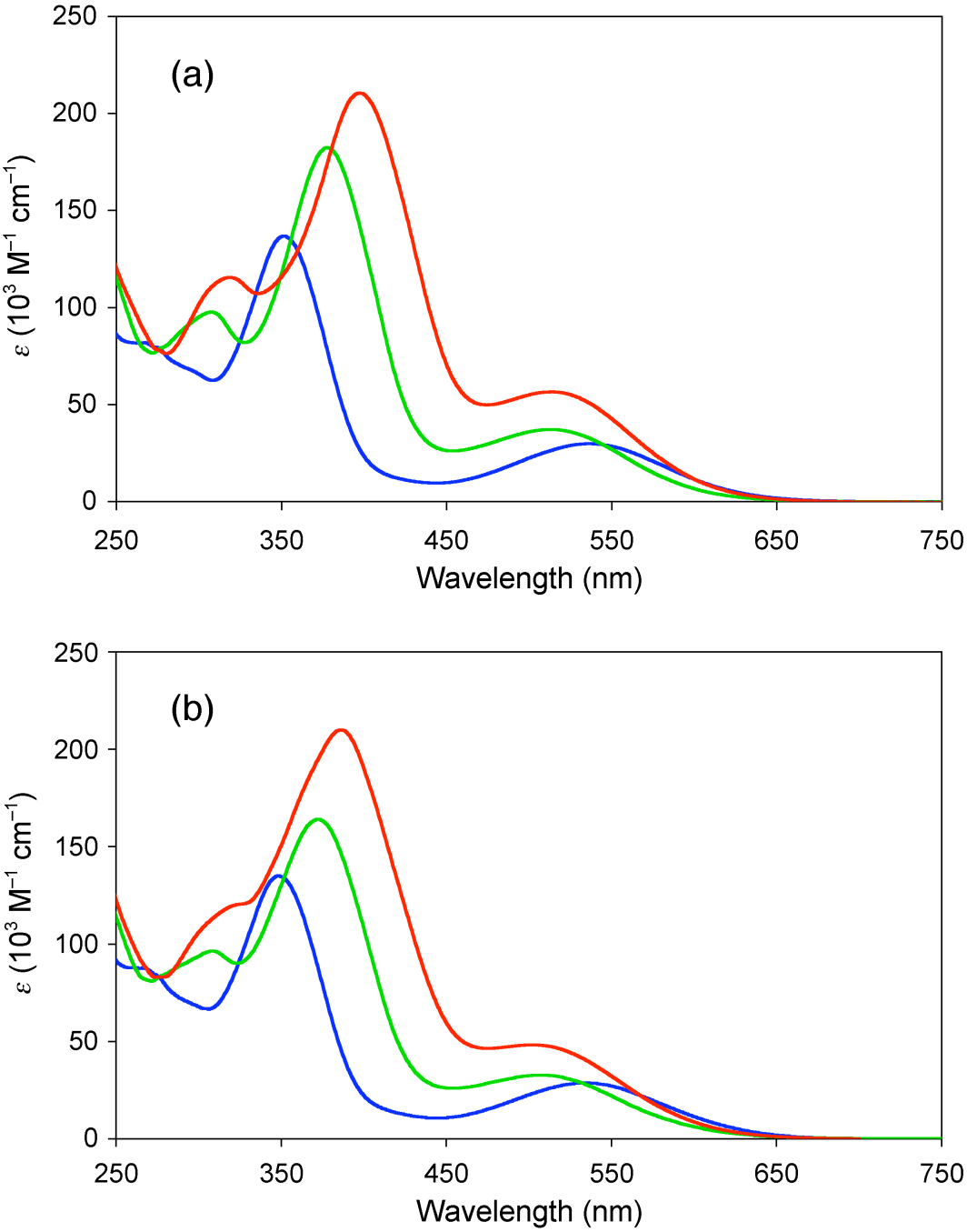

Figure 2. Electronic absorption spectra of (a) **1** (blue), **2** (green) and **3** (red), and (b) **4** (blue), **5** (green) and **6** (red) at 293 K in DCM.

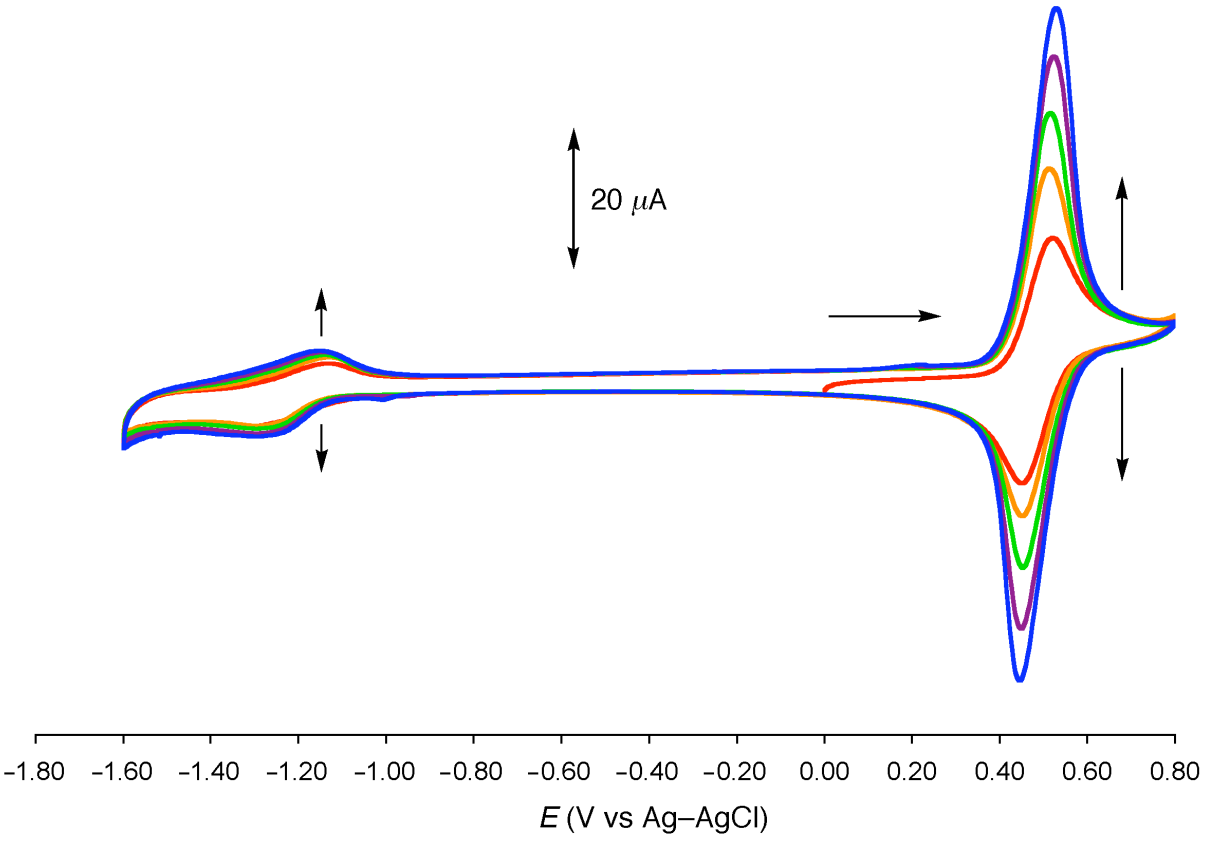

Figure 4. Cyclic voltammograms of **2**, with five sequential scans at 293 K in 1:1 DCM/acetonitrile (glassy-carbon working electrode, scan rate = 100 mV s^{-1}). The single-headed horizontal arrow indicates the direction of the initial scan.

2. Additional Figures and Table

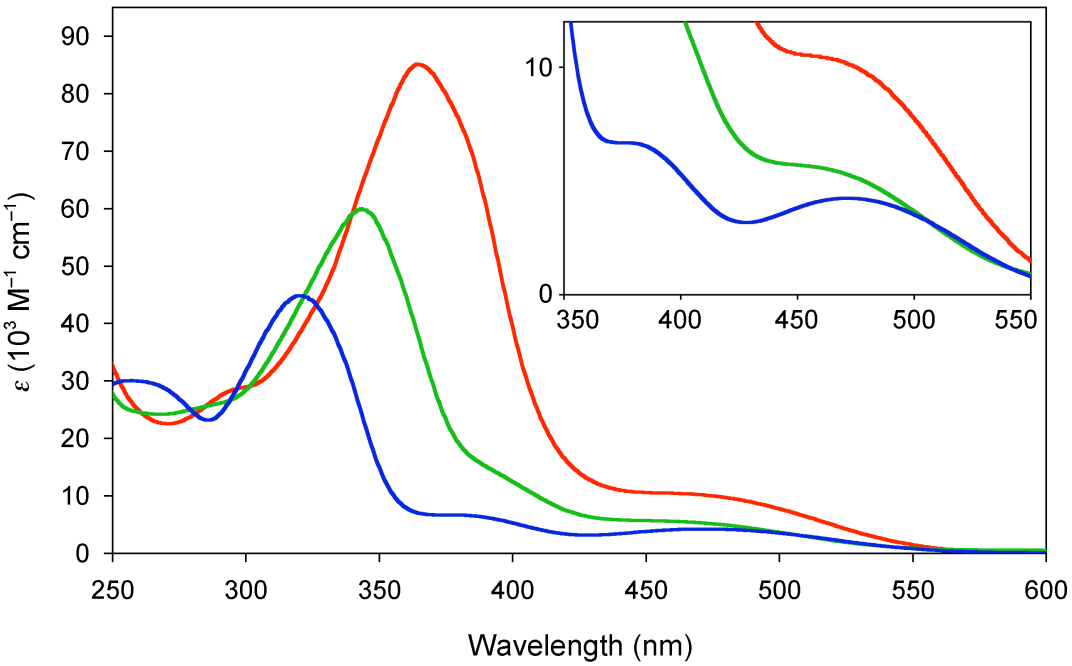

Figure S1. Electronic absorption spectra of Fc_2bpy^A (blue), Fc_2bpy^B (green) and Fc_2bpy^C (red) at 293 K in DCM. The inset shows largely only the MLCT region.

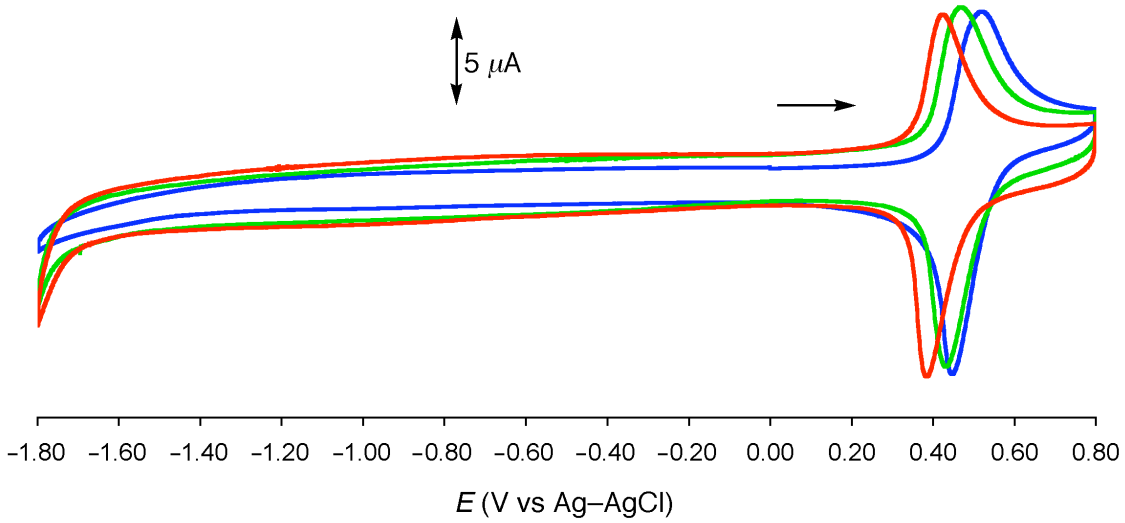

Figure S2. Cyclic voltammograms of Fc_2bpy^A (blue), Fc_2bpy^B (green) and Fc_2bpy^C (red) at 293 K in DCM (glassy-carbon working electrode, scan rate = 100 mV s^{-1}). The single-headed arrow indicates the direction of the initial scans.

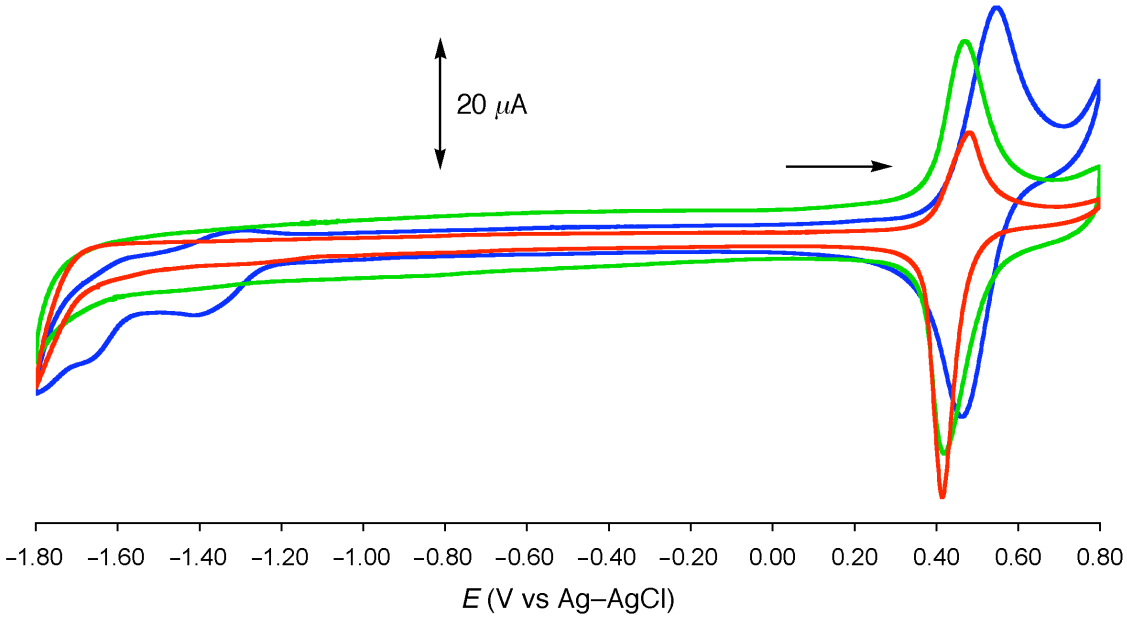

Figure S3. Cyclic voltammograms of **1** (blue), **2** (green) and **3** (red) at 293 K in DCM (glassy-carbon working electrode, scan rate = 100 mV s^{-1}). The concentrations are variable in order to decrease overlap between the traces, and the single-headed arrow indicates the direction of the initial scans.

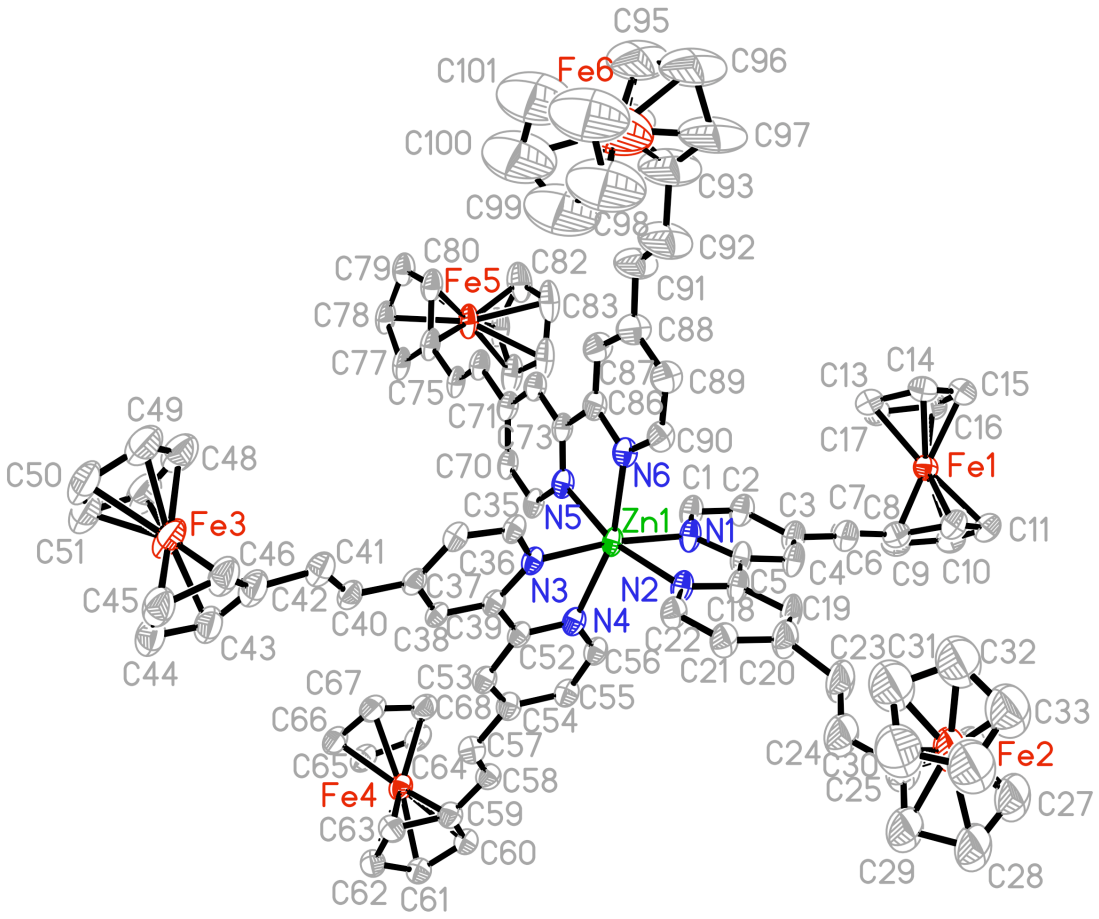

Figure S4. Representation of the molecular structure of the complex dication in the salt **1**•6$MeNO_2$, with the H atoms removed for clarity (30% probability ellipsoids).

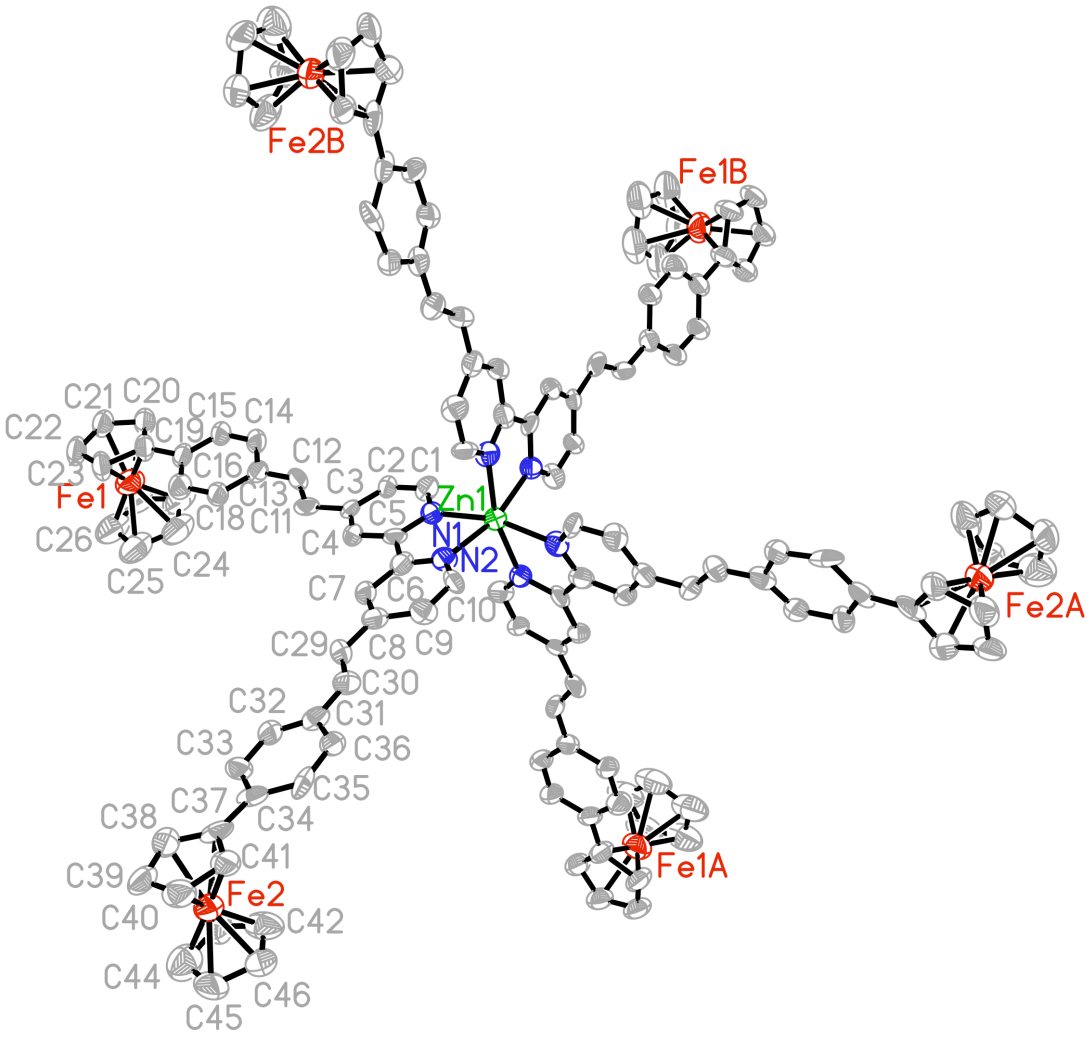

Figure S5. Representation of the molecular structure of the complex dication in the salt **2**•6CH_2Cl_2•1.5C_6H_{14}, with the H atoms removed for clarity (30% probability ellipsoids).

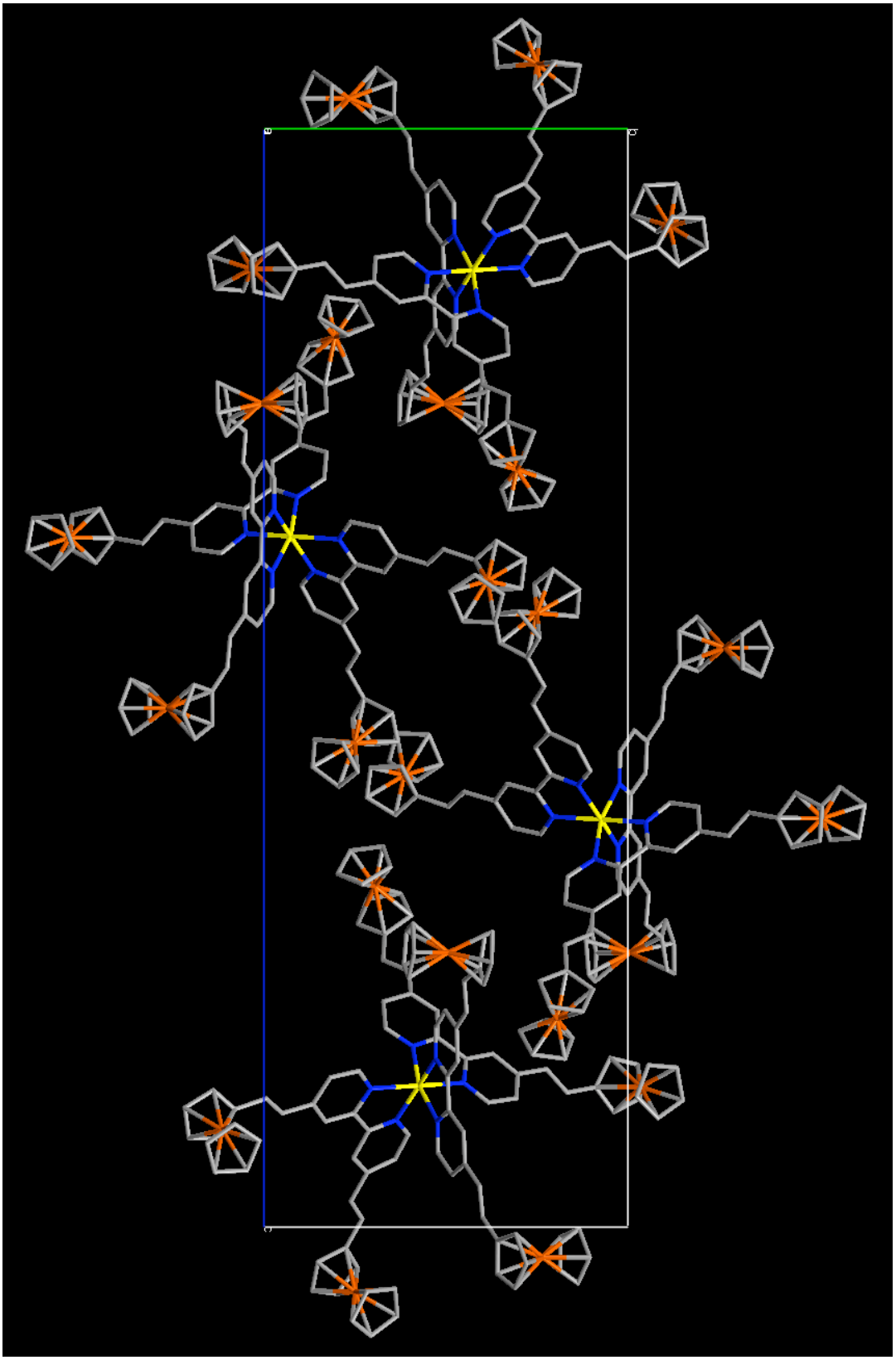

Figure S6. Crystal packing diagram for the salt **1**•6$MeNO_2$, with the H atoms, BPh_4^- anions and solvent molecules removed for clarity (view along the *a* axis).

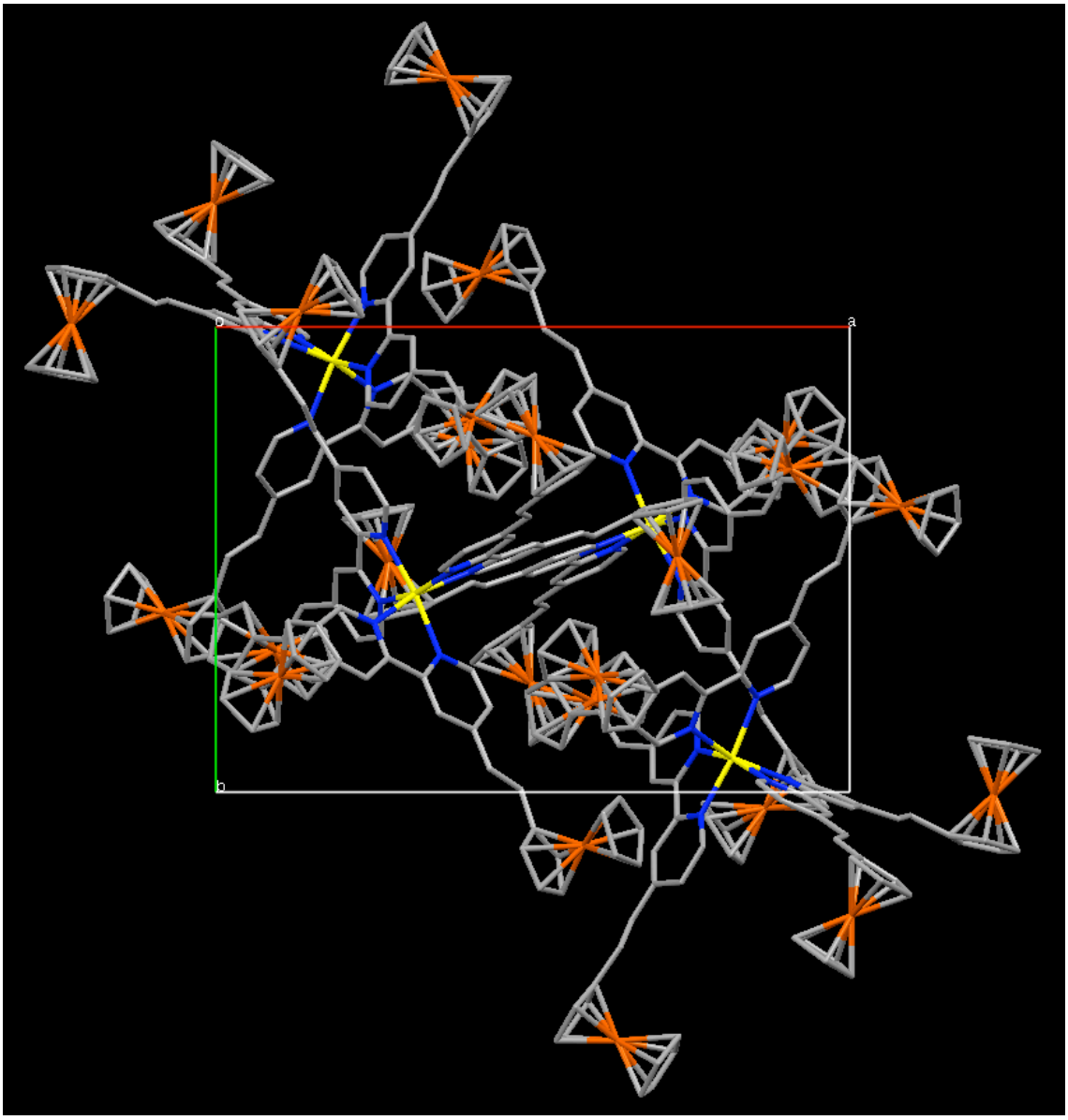

Figure S7. Crystal packing diagram for the salt **1**•6$MeNO_2$, with the H atoms, BPh_4^- anions and solvent molecules removed for clarity (view along the *c* axis).

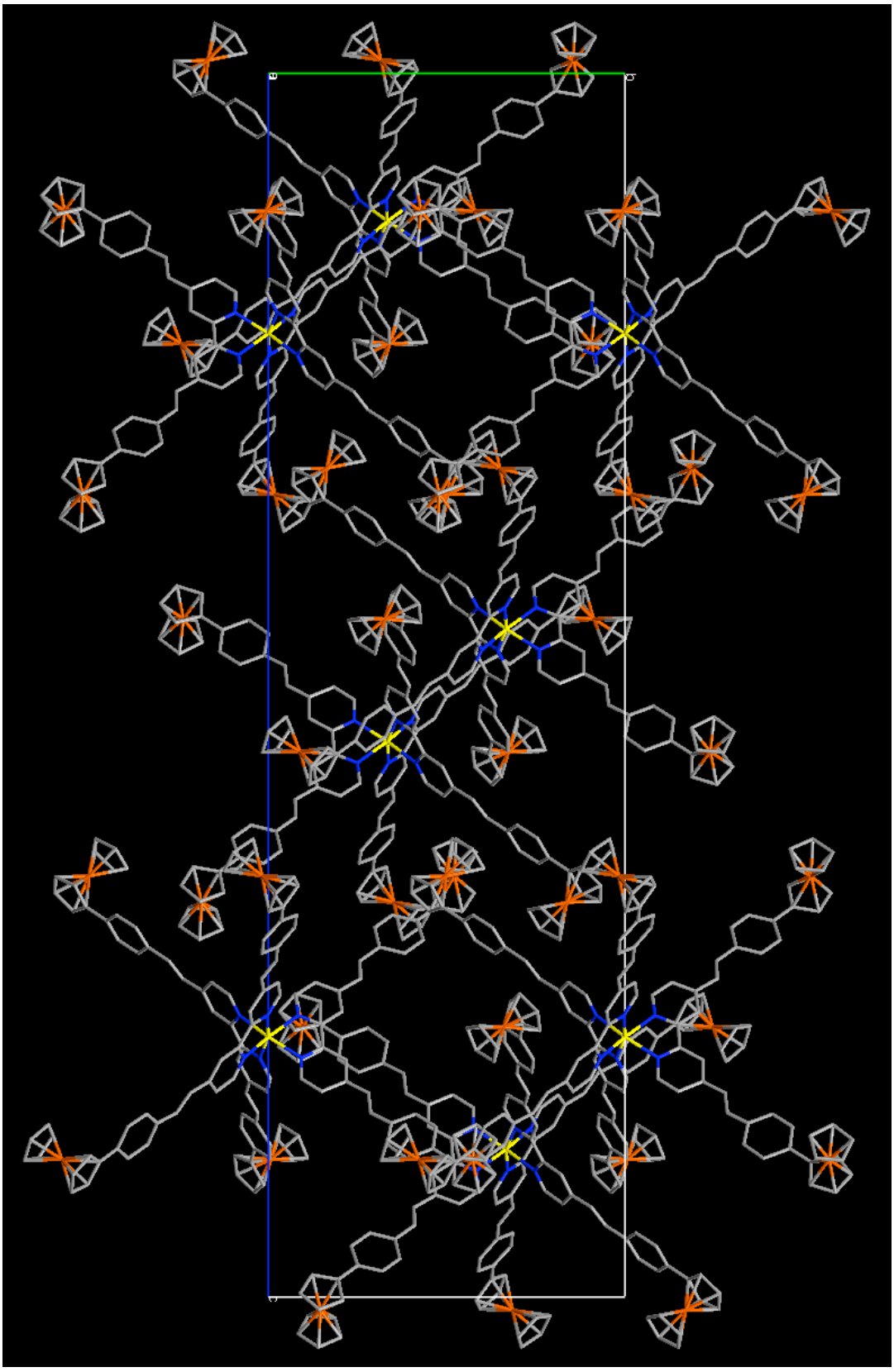

Figure S8. Crystal packing diagram for the salt **2**•6CH_2Cl_2•1.5C_6H_{14}, with the H atoms, BPh_4^- anions and solvent molecules removed for clarity (view along the *a* axis).

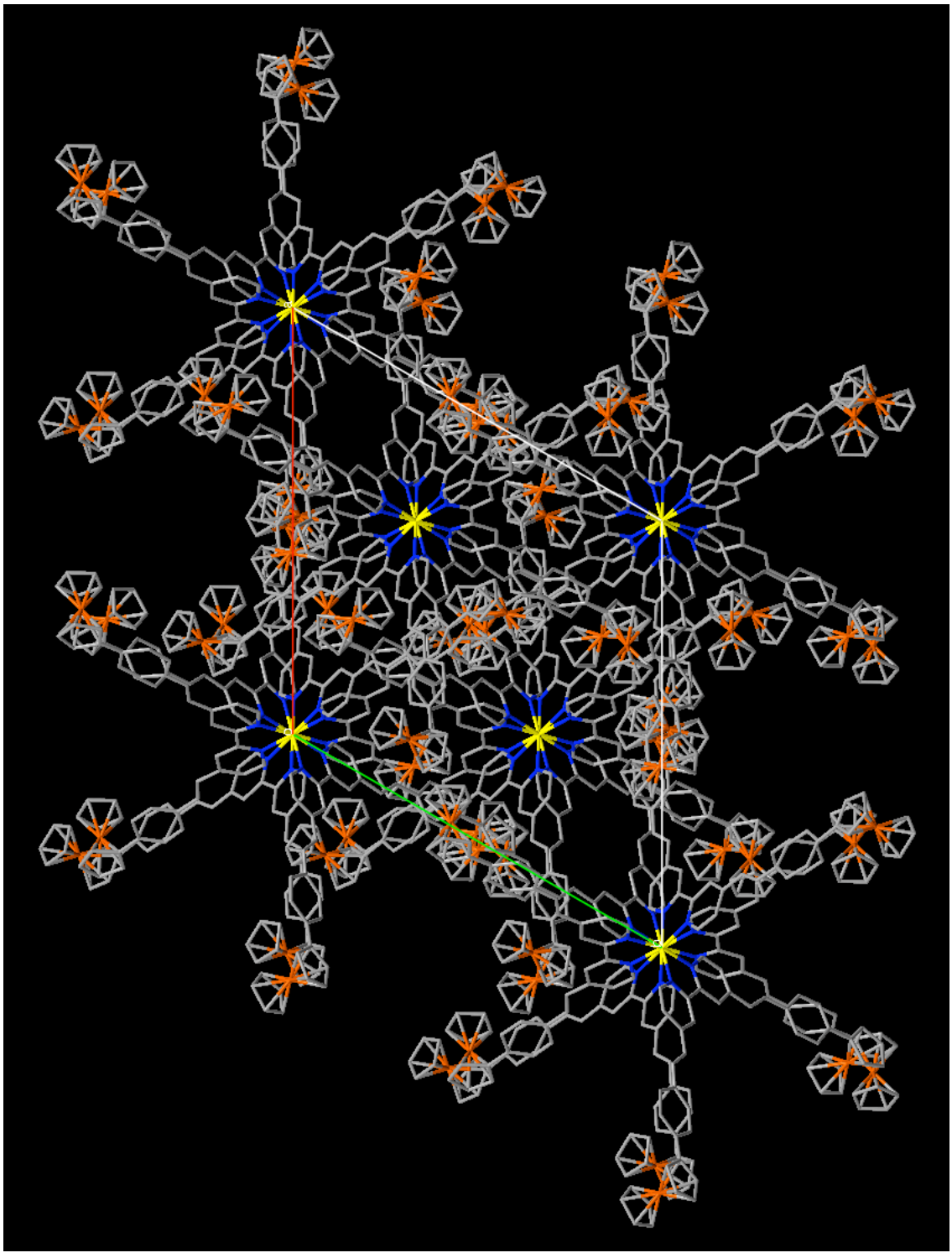

Figure S9. Crystal packing diagram for the salt **2**•6CH_2Cl_2•1.5C_6H_{14}, with the H atoms, BPh_4^- anions and solvent molecules removed for clarity (view along the *c* axis).

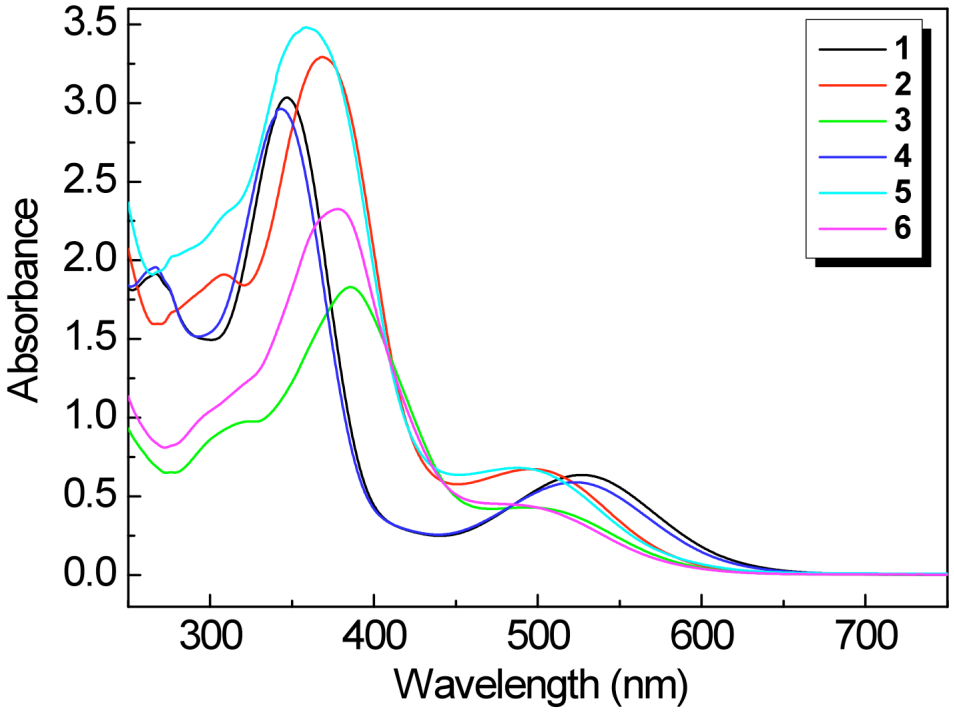

Figure S10. Electronic absorption spectra measured at 293 K in THF.

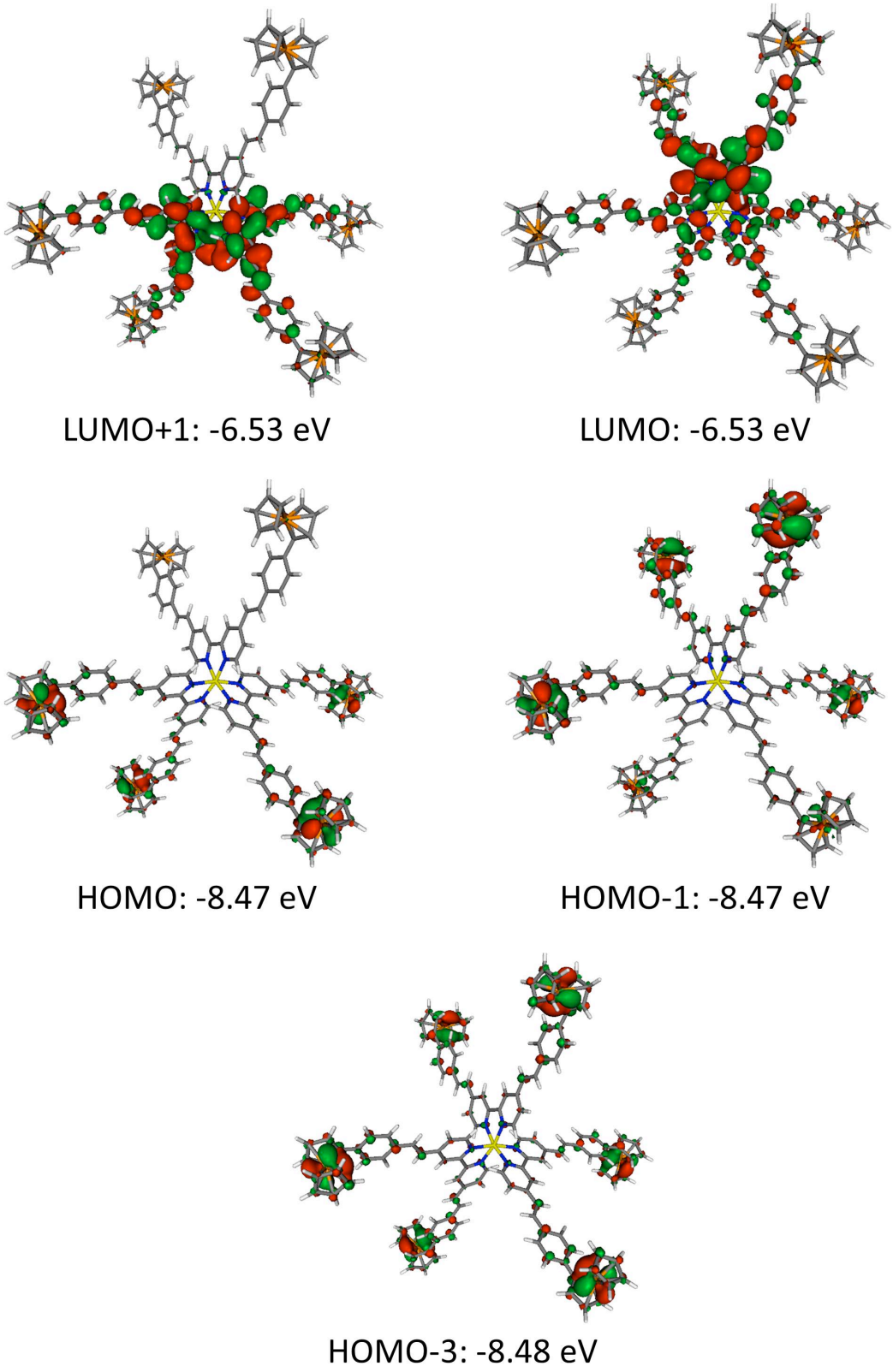

Figure S11. Contour surface diagrams of MOs involved in the MLCT transitions for the complex dication in salt **2** (isosurface value 0.015 au).

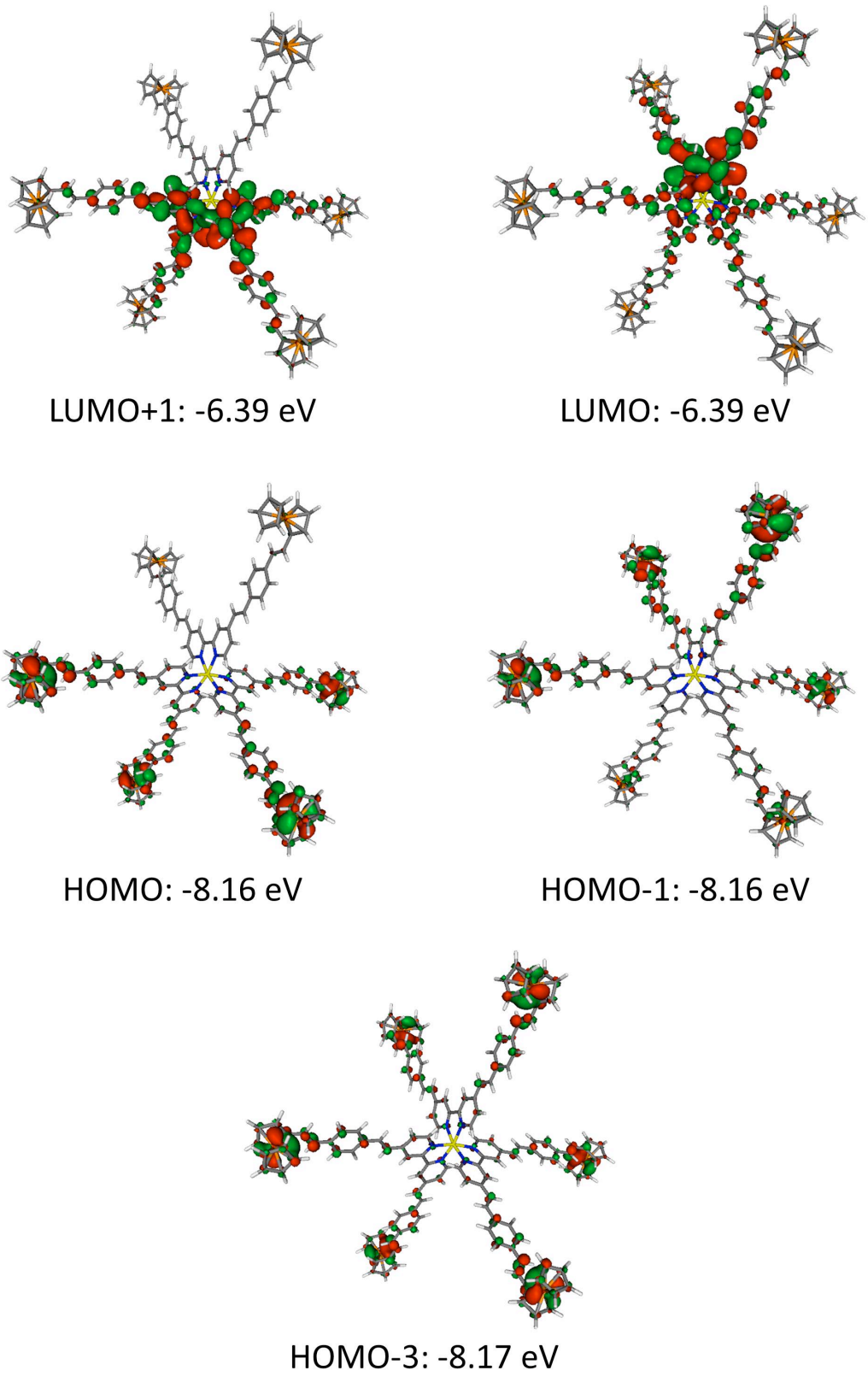

Figure S12. Contour surface diagrams of MOs involved in the MLCT transitions for the complex dication in salt **3** (isosurface value 0.015 au).

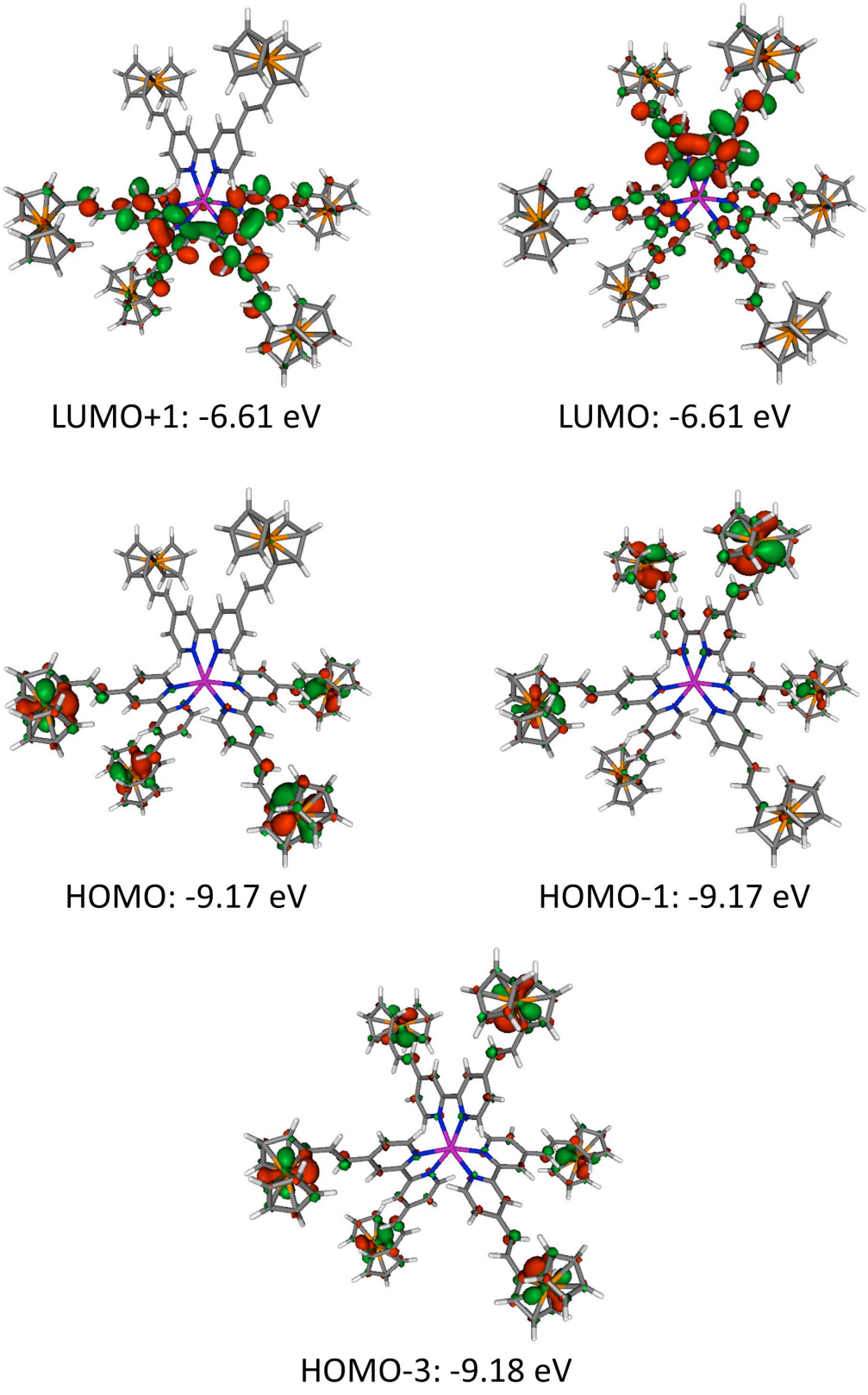

Figure S13. Contour surface diagrams of MOs involved in the MLCT transitions for the complex dication in salt **4** (isosurface value 0.015 au).

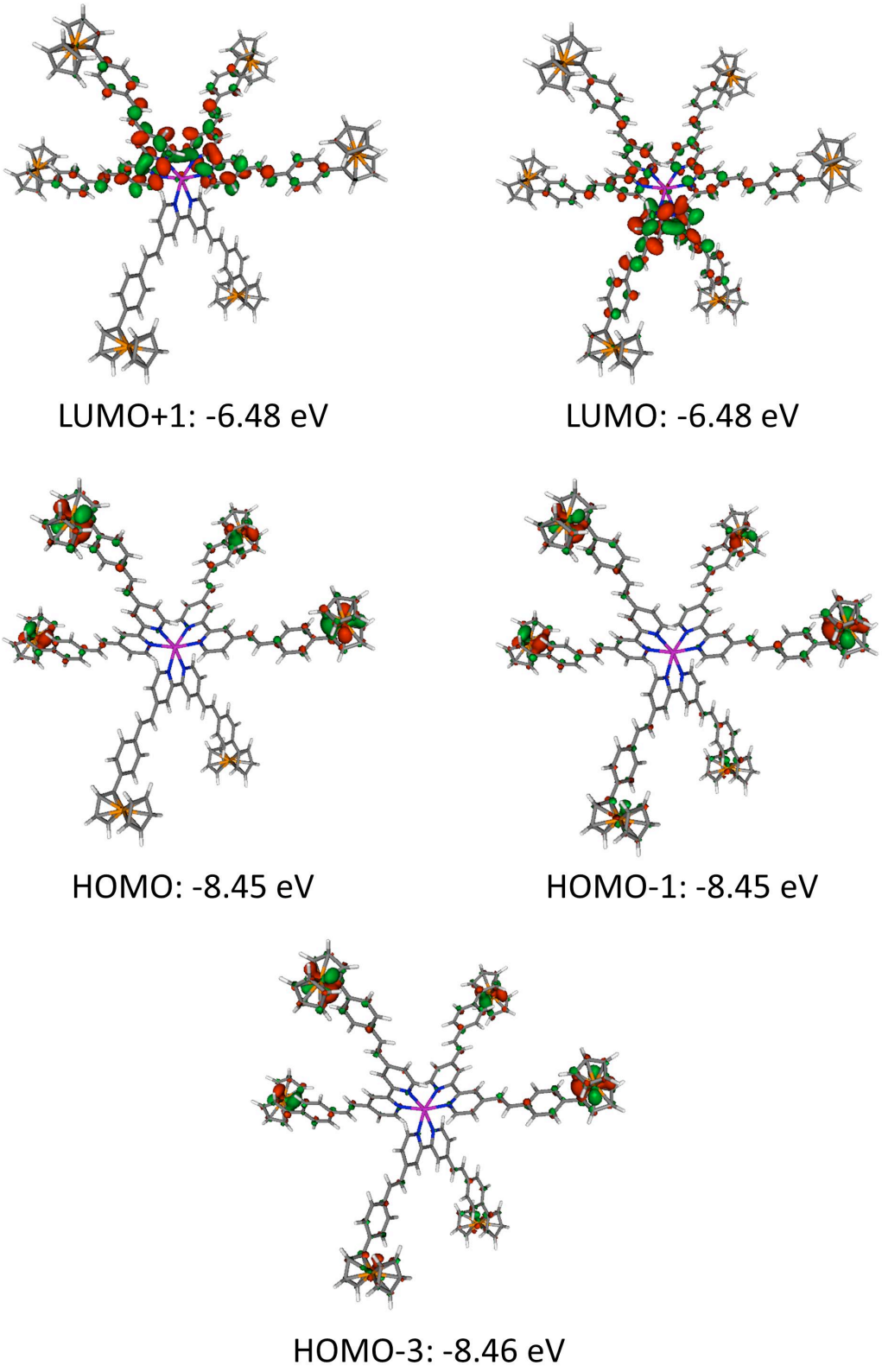

Figure S14. Contour surface diagrams of MOs involved in the MLCT transitions for the complex dication in salt **5** (isosurface value 0.015 au).

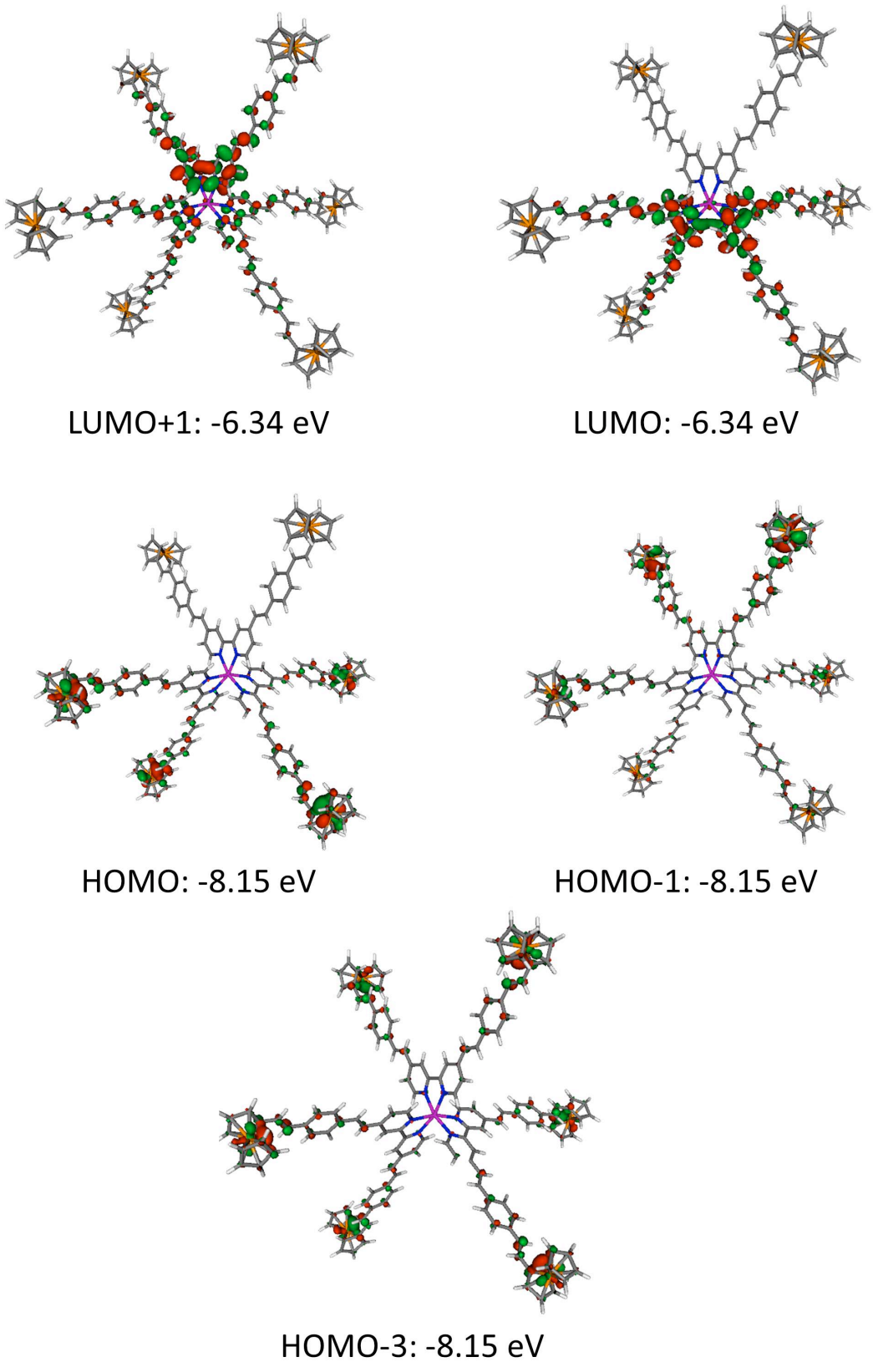

Figure S15. Contour surface diagrams of MOs involved in the MLCT transitions for the complex dication in salt **6** (isosurface value 0.015 au).

Table S1. UV–vis absorption data for the complex salts $[M^{II}(L–L)_3][BPh_4]_2$.

Compound (M/L–L)	λ_{max}[a] [nm]	E_{max}[a] [eV]	Assignment
1 (Zn/Fc_2bpy^A)	526	2.36	d → π^*
	347	3.57	$\pi \rightarrow \pi^*$
2 (Zn/Fc_2bpy^B)	497	2.49	d → π^*
	369	3.36	$\pi \rightarrow \pi^*$
	307	4.04	$\pi \rightarrow \pi^*$
3 (Zn/Fc_2bpy^C)	495	2.51	d → π^*
	385	3.22	$\pi \rightarrow \pi^*$
	320 sh	3.88	$\pi \rightarrow \pi^*$
4 (Cd/Fc_2bpy^A)	523	2.37	d → π^*
	344	3.60	$\pi \rightarrow \pi^*$
5 (Cd/Fc_2bpy^B)	486	2.55	d → π^*
	359	3.45	$\pi \rightarrow \pi^*$
	310 sh	4.00	$\pi \rightarrow \pi^*$
6 (Cd/Fc_2bpy^C)	483	2.57	d → π^*
	378	3.28	$\pi \rightarrow \pi^*$
	320 sh	3.88	$\pi \rightarrow \pi^*$

[a] Solutions in THF with concentrations of ca. 0.3% w/w.

3. Cartesian Coordinates and Energies of Theoretically-Optimized Geometries (B3P86/LanL2DZ)

Dication in 1:

Standard orientation:

Centre Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.594416	1.658571	2.169907
2	6	0	0.463186	2.945129	0.581527
3	6	0	2.182850	2.780454	2.743344
4	1	0	1.798953	0.665375	2.554847
5	6	0	1.029737	4.112236	1.102648
6	6	0	1.915378	4.068169	2.207971
7	1	0	2.847574	2.648584	3.588770
8	1	0	0.811141	5.072604	0.649315
9	6	0	-1.594416	1.658571	-2.169907
10	6	0	-0.463186	2.945129	-0.581527
11	6	0	-2.182850	2.780454	-2.743344
12	1	0	-1.798953	0.665375	-2.554847
13	6	0	-1.029737	4.112236	-1.102648
14	6	0	-1.915378	4.068169	-2.207971
15	1	0	-2.847574	2.648584	-3.588770
16	1	0	-0.811141	5.072604	-0.649315
17	6	0	2.233573	0.551519	-2.169907
18	6	0	2.782150	-1.071434	-0.581527
19	6	0	3.499369	0.500176	-2.743344
20	1	0	1.475708	1.225251	-2.554847
21	6	0	4.076169	-1.164340	-1.102648
22	6	0	4.480827	-0.375319	-2.207971
23	1	0	3.717528	1.141779	-3.588770
24	1	0	4.798574	-1.833833	-0.649315
25	6	0	2.318964	-1.873695	0.581527
26	6	0	0.639157	-2.210090	2.169907
27	6	0	3.046432	-2.947896	1.102648
28	6	0	1.316519	-3.280631	2.743344
29	1	0	-0.323245	-1.890627	2.554847
30	6	0	2.565449	-3.692850	2.207971
31	1	0	3.987434	-3.238771	0.649315
32	1	0	0.869954	-3.790363	3.588770
33	6	0	-0.639157	-2.210090	-2.169907
34	6	0	-2.318964	-1.873695	-0.581527
35	6	0	-1.316519	-3.280631	-2.743344
36	1	0	0.323245	-1.890627	-2.554847
37	6	0	-3.046432	-2.947896	-1.102648
38	6	0	-2.565449	-3.692850	-2.207971
39	1	0	-0.869954	-3.790363	-3.588770
40	1	0	-3.987434	-3.238771	-0.649315
41	6	0	-2.782150	-1.071434	0.581527
42	6	0	-2.233573	0.551519	2.169907
43	6	0	-4.076169	-1.164340	1.102648
44	6	0	-3.499369	0.500176	2.743344
45	1	0	-1.475708	1.225251	2.554847
46	6	0	-4.480827	-0.375319	2.207971
47	1	0	-4.798574	-1.833833	0.649315
48	1	0	-3.717528	1.141779	3.588770
49	7	0	0.748237	1.720444	1.111520
50	7	0	-1.864067	-0.212230	1.111520
51	7	0	-1.115830	-1.508214	-1.111520
52	7	0	1.115830	-1.508214	1.111520

53	7	0	1.864067	-0.212230	-1.111520
54	7	0	-0.748237	1.720444	-1.111520
55	30	0	0.000000	0.000000	0.000000
56	6	0	-5.839766	-0.487817	2.706114
57	6	0	-6.372745	0.232837	3.735468
58	1	0	-6.477270	-1.202429	2.188705
59	1	0	-5.754142	0.969946	4.248307
60	6	0	-3.342345	-4.813477	-2.706114
61	6	0	-2.984730	-5.635378	-3.735468
62	1	0	-4.279969	-5.008266	-2.188705
63	1	0	-2.037073	-5.468206	-4.248307
64	6	0	5.839766	-0.487817	-2.706114
65	6	0	6.372745	0.232837	-3.735468
66	1	0	6.477270	-1.202429	-2.188705
67	1	0	5.754142	0.969946	-4.248307
68	6	0	3.342345	-4.813477	2.706114
69	6	0	2.984730	-5.635378	3.735468
70	1	0	4.279969	-5.008266	2.188705
71	1	0	2.037073	-5.468206	4.248307
72	6	0	2.497421	5.301294	2.706114
73	6	0	3.388015	5.402541	3.735468
74	1	0	2.197301	6.210695	2.188705
75	1	0	3.717069	4.498260	4.248307
76	6	0	-2.497421	5.301294	-2.706114
77	6	0	-3.388015	5.402541	-3.735468
78	1	0	-2.197301	6.210695	-2.188705
79	1	0	-3.717069	4.498260	-4.248307
80	6	0	3.741574	-6.767413	4.214234
81	6	0	5.096470	-7.156853	3.867245
82	6	0	3.264522	-7.715114	5.207576
83	6	0	5.422982	-8.338833	4.608284
84	1	0	2.286679	-7.704436	5.666998
85	6	0	4.293684	-8.684258	5.433000
86	1	0	6.360576	-8.872417	4.566571
87	1	0	4.237836	-9.522876	6.110205
88	1	0	5.747432	-6.654993	3.167047
89	6	0	7.731539	0.143408	-4.214234
90	6	0	8.746251	-0.835246	-3.867245
91	6	0	8.313746	1.030398	-5.207576
92	6	0	9.933132	-0.527024	-4.608284
93	1	0	7.815577	1.871896	-5.666998
94	6	0	9.667630	0.623689	-5.433000
95	1	0	10.864026	-1.072212	-4.566571
96	1	0	10.365971	1.091364	-6.110205
97	1	0	8.637109	-1.649926	-3.167047
98	6	0	3.989964	6.624005	4.214234
99	6	0	3.649781	7.992099	3.867245
100	6	0	5.049224	6.684716	5.207576
101	6	0	4.510150	8.865857	4.608284
102	1	0	5.528898	5.832540	5.666998
103	6	0	5.373946	8.060568	5.433000
104	1	0	4.503450	9.944629	4.566571
105	1	0	6.128134	8.431512	6.110205
106	6	0	-3.989964	6.624005	-4.214234
107	6	0	-3.649781	7.992099	-3.867245
108	6	0	-5.049224	6.684716	-5.207576
109	6	0	-4.510150	8.865857	-4.608284
110	1	0	-5.528898	5.832540	-5.666998
111	6	0	-5.373946	8.060568	-5.433000
112	1	0	-4.503450	9.944629	-4.566571
113	1	0	-6.128134	8.431512	-6.110205
114	1	0	-2.889677	8.304919	-3.167047
115	1	0	2.889677	8.304919	3.167047
116	6	0	-7.731539	0.143408	4.214234
117	6	0	-8.746251	-0.835246	3.867245
118	6	0	-8.313746	1.030398	5.207576
119	6	0	-9.933132	-0.527024	4.608284
120	1	0	-7.815577	1.871896	5.666998

121	6	0	-9.667630	0.623689	5.433000
122	1	0	-10.864026	-1.072212	4.566571
123	1	0	-10.365971	1.091364	6.110205
124	6	0	-3.741574	-6.767413	-4.214234
125	6	0	-5.096470	-7.156853	-3.867245
126	6	0	-3.264522	-7.715114	-5.207576
127	6	0	-5.422982	-8.338833	-4.608284
128	1	0	-2.286679	-7.704436	-5.666998
129	6	0	-4.293684	-8.684258	-5.433000
130	1	0	-6.360576	-8.872417	-4.566571
131	1	0	-4.237836	-9.522876	-6.110205
132	1	0	-5.747432	-6.654993	-3.167047
133	1	0	-8.637109	-1.649926	3.167047
134	26	0	-4.966882	-6.754255	-5.904107
135	26	0	-8.332797	-0.924318	5.904107
136	26	0	3.365915	7.678573	5.904107
137	26	0	-3.365915	7.678573	-5.904107
138	26	0	8.332797	-0.924318	-5.904107
139	26	0	4.966882	-6.754255	5.904107
140	6	0	-4.995828	-4.847638	-6.768152
141	1	0	-4.447083	-3.990615	-6.405675
142	6	0	-4.519555	-5.817817	-7.719391
143	6	0	-6.322090	-5.231729	-6.363013
144	1	0	-3.558407	-5.810294	-8.211316
145	6	0	-5.556311	-6.798274	-7.907650
146	1	0	-6.949969	-4.707659	-5.658063
147	6	0	-6.668932	-6.437626	-7.069643
148	1	0	-5.504468	-7.660470	-8.555462
149	1	0	-7.596766	-6.982510	-6.980624
150	6	0	-6.696092	-1.902695	6.768152
151	1	0	-5.679515	-1.855979	6.405675
152	6	0	-7.298155	-1.005141	7.719391
153	6	0	-7.691855	-2.859226	6.363013
154	1	0	-6.811066	-0.176524	8.211316
155	6	0	-8.665633	-1.412769	7.907650
156	1	0	-7.551937	-3.665020	5.658063
157	6	0	-8.909614	-2.556651	7.069643
158	1	0	-9.386396	-0.936774	8.555462
159	1	0	-9.845414	-3.087737	6.980624
160	6	0	4.995828	-4.847638	6.768152
161	1	0	4.447083	-3.990615	6.405675
162	6	0	4.519555	-5.817817	7.719391
163	6	0	6.322090	-5.231729	6.363013
164	1	0	3.558407	-5.810294	8.211316
165	6	0	5.556311	-6.798274	7.907650
166	1	0	6.949969	-4.707659	5.658063
167	6	0	6.668932	-6.437626	7.069643
168	1	0	5.504468	-7.660470	8.555462
169	1	0	7.596766	-6.982510	6.980624
170	6	0	1.700264	6.750333	6.768152
171	1	0	1.232433	5.846594	6.405675
172	6	0	2.778600	6.822958	7.719391
173	6	0	1.369765	8.090955	6.363013
174	1	0	3.252659	5.986818	8.211316
175	6	0	3.109323	8.211043	7.907650
176	1	0	0.601968	8.372679	5.658063
177	6	0	2.240682	8.994277	7.069643
178	1	0	3.881928	8.597244	8.555462
179	1	0	2.248648	10.070247	6.980624
180	6	0	-1.700264	6.750333	-6.768152
181	1	0	-1.232433	5.846594	-6.405675
182	6	0	-2.778600	6.822958	-7.719391
183	6	0	-1.369765	8.090955	-6.363013
184	1	0	-3.252659	5.986818	-8.211316
185	6	0	-3.109323	8.211043	-7.907650
186	1	0	-0.601968	8.372679	-5.658063
187	6	0	-2.240682	8.994277	-7.069643
188	1	0	-3.881928	8.597244	-8.555462

189	1	0	-2.248648	10.070247	-6.980624
190	6	0	6.696092	-1.902695	-6.768152
191	1	0	5.679515	-1.855979	-6.405675
192	6	0	7.298155	-1.005141	-7.719391
193	6	0	7.691855	-2.859226	-6.363013
194	1	0	6.811066	-0.176524	-8.211316
195	6	0	8.665633	-1.412769	-7.907650
196	1	0	7.551937	-3.665020	-5.658063
197	6	0	8.909614	-2.556651	-7.069643
198	1	0	9.386396	-0.936774	-8.555462
199	1	0	9.845414	-3.087737	-6.980624

E(RB3P86) = -5086.96957095 A.U.

Dication in 2:

Standard orientation:

Centre Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.556418	1.657857	2.196851
2	6	0	0.446778	2.946450	0.594394
3	6	0	2.108544	2.781058	2.802159
4	1	0	1.767887	0.663499	2.574698
5	6	0	0.975851	4.115710	1.149377
6	6	0	1.828011	4.071953	2.280867
7	1	0	2.751299	2.648052	3.664040
8	1	0	0.748224	5.079556	0.708299
9	6	0	-1.556418	1.657857	-2.196851
10	6	0	-0.446778	2.946450	-0.594394
11	6	0	-2.108544	2.781058	-2.802159
12	1	0	-1.767887	0.663499	-2.574698
13	6	0	-0.975851	4.115710	-1.149377
14	6	0	-1.828011	4.071953	-2.280867
15	1	0	-2.751299	2.648052	-3.664040
16	1	0	-0.748224	5.079556	-0.708299
17	6	0	2.213955	0.518969	-2.196851
18	6	0	2.775090	-1.086304	-0.594394
19	6	0	3.462739	0.435524	-2.802159
20	1	0	1.458551	1.199286	-2.574698
21	6	0	4.052235	-1.212743	-1.149377
22	6	0	4.440420	-0.452873	-2.280867
23	1	0	3.668930	1.058669	-3.664040
24	1	0	4.773137	-1.891797	-0.708299
25	6	0	2.328312	-1.860146	0.594394
26	6	0	0.657537	-2.176826	2.196851
27	6	0	3.076384	-2.902967	1.149377
28	6	0	1.354195	-3.216582	2.802159
29	1	0	-0.309336	-1.862785	2.574698
30	6	0	2.612409	-3.619080	2.280867
31	1	0	4.024913	-3.187759	0.708299
32	1	0	0.917631	-3.706721	3.664040
33	6	0	-0.657537	-2.176826	-2.196851
34	6	0	-2.328312	-1.860146	-0.594394
35	6	0	-1.354195	-3.216582	-2.802159
36	1	0	0.309336	-1.862785	-2.574698
37	6	0	-3.076384	-2.902967	-1.149377
38	6	0	-2.612409	-3.619080	-2.280867
39	1	0	-0.917631	-3.706721	-3.664040
40	1	0	-4.024913	-3.187759	-0.708299
41	6	0	-2.775090	-1.086304	0.594394
42	6	0	-2.213955	0.518969	2.196851
43	6	0	-4.052235	-1.212743	1.149377

44	6	0	-3.462739	0.435524	2.802159
45	1	0	-1.458551	1.199286	2.574698
46	6	0	-4.440420	-0.452873	2.280867
47	1	0	-4.773137	-1.891797	0.708299
48	1	0	-3.668930	1.058669	3.664040
49	7	0	0.737505	1.719909	1.117122
50	7	0	-1.858237	-0.221256	1.117122
51	7	0	-1.120732	-1.498653	-1.117122
52	7	0	1.120732	-1.498653	1.117122
53	7	0	1.858237	-0.221256	-1.117122
54	7	0	-0.737505	1.719909	-1.117122
55	30	0	0.000000	0.000000	0.000000
56	6	0	-5.776268	-0.614711	2.826034
57	6	0	-6.283254	0.066336	3.895806
58	1	0	-6.403656	-1.343224	2.316418
59	1	0	-5.645772	0.798300	4.393348
60	6	0	-3.420489	-4.695039	-2.826034
61	6	0	-3.084178	-5.474626	-3.895806
62	1	0	-4.365094	-4.874117	-2.316418
63	1	0	-2.131538	-5.288532	-4.393348
64	6	0	5.776268	-0.614711	-2.826034
65	6	0	6.283254	0.066336	-3.895806
66	1	0	6.403656	-1.343224	-2.316418
67	1	0	5.645772	0.798300	-4.393348
68	6	0	3.420489	-4.695039	2.826034
69	6	0	3.084178	-5.474626	3.895806
70	1	0	4.365094	-4.874117	2.316418
71	1	0	2.131538	-5.288532	4.393348
72	6	0	2.355779	5.309750	2.826034
73	6	0	3.199076	5.408290	3.895806
74	1	0	2.038562	6.217341	2.316418
75	1	0	3.514234	4.490232	4.393348
76	6	0	-2.355779	5.309750	-2.826034
77	6	0	-3.199076	5.408290	-3.895806
78	1	0	-2.038562	6.217341	-2.316418
79	1	0	-3.514234	4.490232	-4.393348
80	6	0	6.012910	-9.837020	6.291646
81	6	0	7.341783	-10.296714	5.936721
82	6	0	5.553167	-10.676333	7.381429
83	6	0	7.676543	-11.408066	6.778269
84	1	0	4.600304	-10.609430	7.884175
85	6	0	6.571828	-11.643013	7.669400
86	1	0	8.601007	-11.964761	6.752368
87	1	0	6.520155	-12.408413	8.428786
88	1	0	7.978603	-9.886823	5.167457
89	6	0	11.525564	-0.288823	-6.291646
90	6	0	12.588107	-1.209814	-5.936721
91	6	0	12.022559	0.528983	-7.381429
92	6	0	13.717946	-0.944048	-6.778269
93	1	0	11.488188	1.320735	-7.884175
94	6	0	13.369059	0.130136	-7.669400
95	1	0	14.662290	-1.466310	-6.752368
96	1	0	14.006078	0.557587	-8.428786
97	1	0	12.551541	-1.966261	-5.167457
98	6	0	5.512654	10.125843	6.291646
99	6	0	5.246324	11.506528	5.936721
100	6	0	6.469392	10.147350	7.381429
101	6	0	6.041403	12.352114	6.778269
102	1	0	6.887884	9.288695	7.884175
103	6	0	6.797231	11.512877	7.669400
104	1	0	6.061283	13.431071	6.752368
105	1	0	7.485923	11.850826	8.428786
106	6	0	-5.512654	10.125843	-6.291646
107	6	0	-5.246324	11.506528	-5.936721
108	6	0	-6.469392	10.147350	-7.381429
109	6	0	-6.041403	12.352114	-6.778269
110	1	0	-6.887884	9.288695	-7.884175
111	6	0	-6.797231	11.512877	-7.669400

112	1	0	-6.061283	13.431071	-6.752368
113	1	0	-7.485923	11.850826	-8.428786
114	1	0	-4.572938	11.853084	-5.167457
115	1	0	4.572938	11.853084	5.167457
116	6	0	-11.525564	-0.288823	6.291646
117	6	0	-12.588107	-1.209814	5.936721
118	6	0	-12.022559	0.528983	7.381429
119	6	0	-13.717946	-0.944048	6.778269
120	1	0	-11.488188	1.320735	7.884175
121	6	0	-13.369059	0.130136	7.669400
122	1	0	-14.662290	-1.466310	6.752368
123	1	0	-14.006078	0.557587	8.428786
124	6	0	-6.012910	-9.837020	-6.291646
125	6	0	-7.341783	-10.296714	-5.936721
126	6	0	-5.553167	-10.676333	-7.381429
127	6	0	-7.676543	-11.408066	-6.778269
128	1	0	-4.600304	-10.609430	-7.884175
129	6	0	-6.571828	-11.643013	-7.669400
130	1	0	-8.601007	-11.964761	-6.752368
131	1	0	-6.520155	-12.408413	-8.428786
132	1	0	-7.978603	-9.886823	-5.167457
133	1	0	-12.551541	-1.966261	5.167457
134	26	0	-7.302807	-9.698851	-7.926948
135	26	0	-12.050855	-1.474991	7.926948
136	26	0	4.748048	11.173842	7.926948
137	26	0	-4.748048	11.173842	-7.926948
138	26	0	12.050855	-1.474991	-7.926948
139	26	0	7.302807	-9.698851	7.926948
140	6	0	-7.393564	-7.709346	-8.560581
141	1	0	-6.853999	-6.892355	-8.104152
142	6	0	-6.912330	-8.549210	-9.626047
143	6	0	-8.704056	-8.171809	-8.185079
144	1	0	-5.958380	-8.461586	-10.124321
145	6	0	-7.927973	-9.529283	-9.911859
146	1	0	-9.330159	-7.751248	-7.412341
147	6	0	-9.034574	-9.296149	-9.021935
148	1	0	-7.866490	-10.309547	-10.655702
149	1	0	-9.947578	-9.871260	-8.982058
150	6	0	-10.373271	-2.548341	8.560581
151	1	0	-9.395954	-2.489560	8.104152
152	6	0	-10.859998	-1.711648	9.626047
153	6	0	-11.429022	-3.452029	8.185079
154	1	0	-10.307138	-0.929315	10.124321
155	6	0	-12.216588	-2.101184	9.911859
156	1	0	-11.377857	-4.204531	7.412341
157	6	0	-12.567988	-3.176096	9.021935
158	1	0	-12.861575	-1.657807	10.655702
159	1	0	-13.522551	-3.679225	8.982058
160	6	0	7.393564	-7.709346	8.560581
161	1	0	6.853999	-6.892355	8.104152
162	6	0	6.912330	-8.549210	9.626047
163	6	0	8.704056	-8.171809	8.185079
164	1	0	5.958380	-8.461586	10.124321
165	6	0	7.927973	-9.529283	9.911859
166	1	0	9.330159	-7.751248	7.412341
167	6	0	9.034574	-9.296149	9.021935
168	1	0	7.866490	-10.309547	10.655702
169	1	0	9.947578	-9.871260	8.982058
170	6	0	2.979708	10.257687	8.560581
171	1	0	2.541955	9.381915	8.104152
172	6	0	3.947668	10.260858	9.626047
173	6	0	2.724966	11.623838	8.185079
174	1	0	4.348758	9.390901	10.124321
175	6	0	4.288615	11.630467	9.911859
176	1	0	2.047698	11.955779	7.412341
177	6	0	3.533414	12.472245	9.021935
178	1	0	4.995085	11.967354	10.655702
179	1	0	3.574973	13.550485	8.982058

180	6	0	-2.979708	10.257687	-8.560581
181	1	0	-2.541955	9.381915	-8.104152
182	6	0	-3.947668	10.260858	-9.626047
183	6	0	-2.724966	11.623838	-8.185079
184	1	0	-4.348758	9.390901	-10.124321
185	6	0	-4.288615	11.630467	-9.911859
186	1	0	-2.047698	11.955779	-7.412341
187	6	0	-3.533414	12.472245	-9.021935
188	1	0	-4.995085	11.967354	-10.655702
189	1	0	-3.574973	13.550485	-8.982058
190	6	0	10.373271	-2.548341	-8.560581
191	1	0	9.395954	-2.489560	-8.104152
192	6	0	10.859998	-1.711648	-9.626047
193	6	0	11.429022	-3.452029	-8.185079
194	1	0	10.307138	-0.929315	-10.124321
195	6	0	12.216588	-2.101184	-9.911859
196	1	0	11.377857	-4.204531	-7.412341
197	6	0	12.567988	-3.176096	-9.021935
198	1	0	12.861575	-1.657807	-10.655702
199	1	0	13.522551	-3.679225	-8.982058
200	6	0	3.858046	-6.559633	4.471230
201	6	0	3.325339	-7.267269	5.576279
202	6	0	5.127123	-6.963905	3.985927
203	6	0	4.017502	-8.321573	6.166779
204	1	0	2.351614	-6.982029	5.969071
205	6	0	5.817753	-8.016302	4.576611
206	1	0	5.575055	-6.454294	3.137624
207	6	0	5.285273	-8.723278	5.684851
208	1	0	3.575031	-8.840568	7.010416
209	1	0	6.783071	-8.306800	4.175132
210	6	0	7.609832	-0.061349	-4.471230
211	6	0	8.594480	-0.958266	-3.985927
212	6	0	7.956309	0.753806	-5.576279
213	6	0	9.851198	-1.030171	-4.576611
214	1	0	8.377110	-1.600992	-3.137624
215	6	0	9.215445	0.681528	-6.166779
216	1	0	7.222421	1.454457	-5.969071
217	6	0	10.197217	-0.215542	-5.684851
218	1	0	10.585435	-1.720912	-4.175132
219	1	0	9.443672	1.324216	-7.010416
220	6	0	3.751786	6.620982	4.471230
221	6	0	4.630970	6.513463	5.576279
222	6	0	3.467357	7.922171	3.985927
223	6	0	5.197943	7.640045	6.166779
224	1	0	4.870807	5.527572	5.969071
225	6	0	4.033445	9.046473	4.576611
226	1	0	2.802055	8.055286	3.137624
227	6	0	4.911944	8.938820	5.684851
228	1	0	5.868641	7.516352	7.010416
229	1	0	3.802364	10.027712	4.175132
230	6	0	-3.751786	6.620982	-4.471230
231	6	0	-3.467357	7.922171	-3.985927
232	6	0	-4.630970	6.513463	-5.576279
233	6	0	-4.033445	9.046473	-4.576611
234	1	0	-2.802055	8.055286	-3.137624
235	6	0	-5.197943	7.640045	-6.166779
236	1	0	-4.870807	5.527572	-5.969071
237	6	0	-4.911944	8.938820	-5.684851
238	1	0	-3.802364	10.027712	-4.175132
239	1	0	-5.868641	7.516352	-7.010416
240	6	0	-7.609832	-0.061349	4.471230
241	6	0	-7.956309	0.753806	5.576279
242	6	0	-8.594480	-0.958266	3.985927
243	6	0	-9.215445	0.681528	6.166779
244	1	0	-7.222421	1.454457	5.969071
245	6	0	-9.851198	-1.030171	4.576611
246	1	0	-8.377110	-1.600992	3.137624
247	6	0	-10.197217	-0.215542	5.684851

248	1	0	-9.443672	1.324216	7.010416
249	1	0	-10.585435	-1.720912	4.175132
250	6	0	-3.858046	-6.559633	-4.471230
251	6	0	-5.127123	-6.963905	-3.985927
252	6	0	-3.325339	-7.267269	-5.576279
253	6	0	-5.817753	-8.016302	-4.576611
254	1	0	-5.575055	-6.454294	-3.137624
255	6	0	-4.017502	-8.321573	-6.166779
256	1	0	-2.351614	-6.982029	-5.969071
257	6	0	-5.285273	-8.723278	-5.684851
258	1	0	-6.783071	-8.306800	-4.175132
259	1	0	-3.575031	-8.840568	-7.010416

E(RB3P86) = -6477.45083937 A.U.

Dication in 3:

Standard orientation:

Centre Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.553320	1.656092	2.197317
2	6	0	0.444733	2.947677	0.595965
3	6	0	2.101334	2.778289	2.807415
4	1	0	1.767217	0.660506	2.570668
5	6	0	0.969143	4.116455	1.156381
6	6	0	1.817571	4.070964	2.291018
7	1	0	2.744513	2.643343	3.668739
8	1	0	0.739721	5.081278	0.718191
9	6	0	-1.553320	1.656092	-2.197317
10	6	0	-0.444733	2.947677	-0.595965
11	6	0	-2.101334	2.778289	-2.807415
12	1	0	-1.767217	0.660506	-2.570668
13	6	0	-0.969143	4.116455	-1.156381
14	6	0	-1.817571	4.070964	-2.291018
15	1	0	-2.744513	2.643343	-3.668739
16	1	0	-0.739721	5.081278	-0.718191
17	6	0	2.210878	0.517169	-2.197317
18	6	0	2.775130	-1.088688	-0.595965
19	6	0	3.456736	0.430664	-2.807415
20	1	0	1.455623	1.200202	-2.570668
21	6	0	4.049526	-1.218925	-1.156381
22	6	0	4.434344	-0.461419	-2.291018
23	1	0	3.661459	1.055146	-3.668739
24	1	0	4.770376	-1.900022	-0.718191
25	6	0	2.330397	-1.858989	0.595965
26	6	0	0.657558	-2.173261	2.197317
27	6	0	3.080383	-2.897530	1.156381
28	6	0	1.355402	-3.208953	2.807415
29	1	0	-0.311594	-1.860708	2.570668
30	6	0	2.616773	-3.609545	2.291018
31	1	0	4.030655	-3.181256	0.718191
32	1	0	0.916946	-3.698489	3.668739
33	6	0	-0.657558	-2.173261	-2.197317
34	6	0	-2.330397	-1.858989	-0.595965
35	6	0	-1.355402	-3.208953	-2.807415
36	1	0	0.311594	-1.860708	-2.570668
37	6	0	-3.080383	-2.897530	-1.156381
38	6	0	-2.616773	-3.609545	-2.291018
39	1	0	-0.916946	-3.698489	-3.668739
40	1	0	-4.030655	-3.181256	-0.718191
41	6	0	-2.775130	-1.088688	0.595965
42	6	0	-2.210878	0.517169	2.197317
43	6	0	-4.049526	-1.218925	1.156381

44	6	0	-3.456736	0.430664	2.807415
45	1	0	-1.455623	1.200202	2.570668
46	6	0	-4.434344	-0.461419	2.291018
47	1	0	-4.770376	-1.900022	0.718191
48	1	0	-3.661459	1.055146	3.668739
49	7	0	0.736063	1.720121	1.116515
50	7	0	-1.857700	-0.222611	1.116515
51	7	0	-1.121637	-1.497510	-1.116515
52	7	0	1.121637	-1.497510	1.116515
53	7	0	1.857700	-0.222611	-1.116515
54	7	0	-0.736063	1.720121	-1.116515
55	30	0	0.000000	0.000000	0.000000
56	6	0	-5.765561	-0.626623	2.844739
57	6	0	-6.257384	0.039116	3.932195
58	1	0	-6.400931	-1.345739	2.331658
59	1	0	-5.608033	0.756197	4.435939
60	6	0	-3.425452	-4.679811	-2.844739
61	6	0	-3.094817	-5.438611	-3.932195
62	1	0	-4.365910	-4.870499	-2.331658
63	1	0	-2.149131	-5.234798	-4.435939
64	6	0	5.765561	-0.626623	-2.844739
65	6	0	6.257384	0.039116	-3.932195
66	1	0	6.400931	-1.345739	-2.331658
67	1	0	5.608033	0.756197	-4.435939
68	6	0	3.425452	-4.679811	2.844739
69	6	0	3.094817	-5.438611	3.932195
70	1	0	4.365910	-4.870499	2.331658
71	1	0	2.149131	-5.234798	4.435939
72	6	0	2.340109	5.306434	2.844739
73	6	0	3.162567	5.399496	3.932195
74	1	0	2.035021	6.216238	2.331658
75	1	0	3.458902	4.478601	4.435939
76	6	0	-2.340109	5.306434	-2.844739
77	6	0	-3.162567	5.399496	-3.932195
78	1	0	-2.035021	6.216238	-2.331658
79	1	0	-3.458902	4.478601	-4.435939
80	6	0	6.481902	-11.574826	8.020872
81	6	0	7.853770	-11.945958	7.732976
82	6	0	6.010051	-12.463038	9.066465
83	6	0	8.200243	-13.061640	8.565593
84	1	0	5.022129	-12.446015	9.503726
85	6	0	7.062293	-13.381861	9.388123
86	1	0	9.154663	-13.566136	8.582154
87	1	0	7.012632	-14.172604	10.121150
88	1	0	8.505988	-11.470611	7.015485
89	6	0	13.265044	0.173921	-8.020872
90	6	0	14.272388	-0.828585	-7.732976
91	6	0	13.798333	1.026662	-9.066465
92	6	0	15.411834	-0.570799	-8.565593
93	1	0	13.289630	1.873716	-9.503726
94	6	0	15.120178	0.574805	-9.388123
95	1	0	16.325950	-1.145103	-8.582154
96	1	0	15.780151	1.013184	-10.121150
97	1	0	14.186835	-1.631096	-7.015485
98	6	0	6.783142	11.400905	8.020872
99	6	0	6.418618	12.774543	7.732976
100	6	0	7.788282	11.436376	9.066465
101	6	0	7.211591	13.632439	8.565593
102	1	0	8.267501	10.572299	9.503726
103	6	0	8.057885	12.807056	9.388123
104	1	0	7.171287	14.711239	8.582154
105	1	0	8.767519	13.159420	10.121150
106	6	0	-6.783142	11.400905	-8.020872
107	6	0	-6.418618	12.774543	-7.732976
108	6	0	-7.788282	11.436376	-9.066465
109	6	0	-7.211591	13.632439	-8.565593
110	1	0	-8.267501	10.572299	-9.503726
111	6	0	-8.057885	12.807056	-9.388123

112	1	0	-7.171287	14.711239	-8.582154
113	1	0	-8.767519	13.159420	-10.121150
114	1	0	-5.680846	13.101707	-7.015485
115	1	0	5.680846	13.101707	7.015485
116	6	0	-13.265044	0.173921	8.020872
117	6	0	-14.272388	-0.828585	7.732976
118	6	0	-13.798333	1.026662	9.066465
119	6	0	-15.411834	-0.570799	8.565593
120	1	0	-13.289630	1.873716	9.503726
121	6	0	-15.120178	0.574805	9.388123
122	1	0	-16.325950	-1.145103	8.582154
123	1	0	-15.780151	1.013184	10.121150
124	6	0	-6.481902	-11.574826	-8.020872
125	6	0	-7.853770	-11.945958	-7.732976
126	6	0	-6.010051	-12.463038	-9.066465
127	6	0	-8.200243	-13.061640	-8.565593
128	1	0	-5.022129	-12.446015	-9.503726
129	6	0	-7.062293	-13.381861	-9.388123
130	1	0	-9.154663	-13.566136	-8.582154
131	1	0	-7.012632	-14.172604	-10.121150
132	1	0	-8.505988	-11.470611	-7.015485
133	1	0	-14.186835	-1.631096	7.015485
134	26	0	-7.670615	-11.410391	-9.736077
135	26	0	-13.716996	-0.937752	9.736077
136	26	0	6.046381	12.348143	9.736077
137	26	0	-6.046381	12.348143	-9.736077
138	26	0	13.716996	-0.937752	-9.736077
139	26	0	7.670615	-11.410391	9.736077
140	6	0	-7.588267	-9.445994	-10.449981
141	1	0	-7.001961	-8.652784	-10.009764
142	6	0	-7.145248	-10.363867	-11.466993
143	6	0	-8.939470	-9.791278	-10.095157
144	1	0	-6.174523	-10.370536	-11.939945
145	6	0	-8.226262	-11.273228	-11.745258
146	1	0	-9.550338	-9.292120	-9.357881
147	6	0	-9.334339	-10.920485	-10.897337
148	1	0	-8.205312	-12.085497	-12.456463
149	1	0	-10.290504	-11.421036	-10.863395
150	6	0	-11.974604	-1.848635	10.449981
151	1	0	-10.994511	-1.737484	10.009764
152	6	0	-12.547996	-1.006033	11.466993
153	6	0	-12.949231	-2.846169	10.095157
154	1	0	-12.068409	-0.162026	11.939945
155	6	0	-13.876033	-1.487538	11.745258
156	1	0	-12.822381	-3.624775	9.357881
157	6	0	-14.124587	-2.623532	10.897337
158	1	0	-14.569003	-1.063260	12.456463
159	1	0	-15.036159	-3.201320	10.863395
160	6	0	7.588267	-9.445994	10.449981
161	1	0	7.001961	-8.652784	10.009764
162	6	0	7.145248	-10.363867	11.466993
163	6	0	8.939470	-9.791278	10.095157
164	1	0	6.174523	-10.370536	11.939945
165	6	0	8.226262	-11.273228	11.745258
166	1	0	9.550338	-9.292120	9.357881
167	6	0	9.334339	-10.920485	10.897337
168	1	0	8.205312	-12.085497	12.456463
169	1	0	10.290504	-11.421036	10.863395
170	6	0	4.386337	11.294629	10.449981
171	1	0	3.992550	10.390268	10.009764
172	6	0	5.402748	11.369900	11.466993
173	6	0	4.009761	12.637447	10.095157
174	1	0	5.893886	10.532562	11.939945
175	6	0	5.649771	12.760766	11.745258
176	1	0	3.272043	12.916895	9.357881
177	6	0	4.790248	13.544017	10.897337
178	1	0	6.363692	13.148757	12.456463
179	1	0	4.745655	14.622356	10.863395

180	6	0	-4.386337	11.294629	-10.449981
181	1	0	-3.992550	10.390268	-10.009764
182	6	0	-5.402748	11.369900	-11.466993
183	6	0	-4.009761	12.637447	-10.095157
184	1	0	-5.893886	10.532562	-11.939945
185	6	0	-5.649771	12.760766	-11.745258
186	1	0	-3.272043	12.916895	-9.357881
187	6	0	-4.790248	13.544017	-10.897337
188	1	0	-6.363692	13.148757	-12.456463
189	1	0	-4.745655	14.622356	-10.863395
190	6	0	11.974604	-1.848635	-10.449981
191	1	0	10.994511	-1.737484	-10.009764
192	6	0	12.547996	-1.006033	-11.466993
193	6	0	12.949231	-2.846169	-10.095157
194	1	0	12.068409	-0.162026	-11.939945
195	6	0	13.876033	-1.487538	-11.745258
196	1	0	12.822381	-3.624775	-9.357881
197	6	0	14.124587	-2.623532	-10.897337
198	1	0	14.569003	-1.063260	-12.456463
199	1	0	15.036159	-3.201320	-10.863395
200	6	0	3.865930	-6.516261	4.521243
201	6	0	3.346296	-7.183560	5.660328
202	6	0	5.120566	-6.950907	4.023936
203	6	0	4.033322	-8.225479	6.273470
204	1	0	2.384889	-6.870196	6.062137
205	6	0	5.806844	-7.993196	4.636450
206	1	0	5.559675	-6.471784	3.153597
207	6	0	5.288380	-8.663027	5.777179
208	1	0	3.595323	-8.706234	7.142230
209	1	0	6.766052	-8.311409	4.235847
210	6	0	7.576213	-0.089863	-4.521243
211	6	0	8.579945	-0.959087	-4.023936
212	6	0	7.894293	0.693803	-5.660328
213	6	0	9.825733	-1.032276	-4.636450
214	1	0	8.384567	-1.578928	-3.153597
215	6	0	9.140135	0.619780	-6.273470
216	1	0	7.142209	1.369724	-6.062137
217	6	0	10.146591	-0.248358	-5.777179
218	1	0	10.580917	-1.703868	-4.235847
219	1	0	9.337481	1.239476	-7.142230
220	6	0	3.710283	6.606124	4.521243
221	6	0	4.547997	6.489757	5.660328
222	6	0	3.459379	7.909994	4.023936
223	6	0	5.106813	7.605699	6.273470
224	1	0	4.757320	5.500473	6.062137
225	6	0	4.018889	9.025472	4.636450
226	1	0	2.824892	8.050712	3.153597
227	6	0	4.858211	8.911385	5.777179
228	1	0	5.742158	7.466758	7.142230
229	1	0	3.814865	10.015277	4.235847
230	6	0	-3.710283	6.606124	-4.521243
231	6	0	-3.459379	7.909994	-4.023936
232	6	0	-4.547997	6.489757	-5.660328
233	6	0	-4.018889	9.025472	-4.636450
234	1	0	-2.824892	8.050712	-3.153597
235	6	0	-5.106813	7.605699	-6.273470
236	1	0	-4.757320	5.500473	-6.062137
237	6	0	-4.858211	8.911385	-5.777179
238	1	0	-3.814865	10.015277	-4.235847
239	1	0	-5.742158	7.466758	-7.142230
240	6	0	-7.576213	-0.089863	4.521243
241	6	0	-7.894293	0.693803	5.660328
242	6	0	-8.579945	-0.959087	4.023936
243	6	0	-9.140135	0.619780	6.273470
244	1	0	-7.142209	1.369724	6.062137
245	6	0	-9.825733	-1.032276	4.636450
246	1	0	-8.384567	-1.578928	3.153597
247	6	0	-10.146591	-0.248358	5.777179

248	1	0	-9.337481	1.239476	7.142230
249	1	0	-10.580917	-1.703868	4.235847
250	6	0	-3.865930	-6.516261	-4.521243
251	6	0	-5.120566	-6.950907	-4.023936
252	6	0	-3.346296	-7.183560	-5.660328
253	6	0	-5.806844	-7.993196	-4.636450
254	1	0	-5.559675	-6.471784	-3.153597
255	6	0	-4.033322	-8.225479	-6.273470
256	1	0	-2.384889	-6.870196	-6.062137
257	6	0	-5.288380	-8.663027	-5.777179
258	1	0	-6.766052	-8.311409	-4.235847
259	1	0	-3.595323	-8.706234	-7.142230
260	6	0	6.059565	-9.749123	6.365577
261	6	0	5.703483	-10.496470	7.447730
262	1	0	7.005553	-9.973019	5.874125
263	1	0	4.750921	-10.305160	7.941744
264	6	0	-6.059565	-9.749123	-6.365577
265	6	0	-5.703483	-10.496470	-7.447730
266	1	0	-7.005553	-9.973019	-5.874125
267	1	0	-4.750921	-10.305160	-7.941744
268	6	0	-11.472771	-0.373176	6.365577
269	6	0	-11.941951	0.308874	7.447730
270	1	0	-12.139664	-1.080477	5.874125
271	1	0	-11.299991	1.038162	7.941744
272	6	0	-5.413206	10.122299	-6.365577
273	6	0	-6.238468	10.187596	-7.447730
274	1	0	-5.134111	11.053496	-5.874125
275	1	0	-6.549070	9.266998	-7.941744
276	6	0	5.413206	10.122299	6.365577
277	6	0	6.238468	10.187596	7.447730
278	1	0	5.134111	11.053496	5.874125
279	1	0	6.549070	9.266998	7.941744
280	6	0	11.472771	-0.373176	-6.365577
281	6	0	11.941951	0.308874	-7.447730
282	1	0	12.139664	-1.080477	-5.874125
283	1	0	11.299991	1.038162	-7.941744

E(RB3P86) = -6943.32404468 A.U.

Dication in 4:

Standard orientation:

Centre Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.600348	1.883225	2.203400
2	6	0	0.470631	3.127262	0.577887
3	6	0	2.210859	3.014824	2.732466
4	1	0	1.797335	0.901377	2.621707
5	6	0	1.064847	4.302019	1.052481
6	6	0	1.958015	4.285394	2.152164
7	1	0	2.880168	2.902786	3.577136
8	1	0	0.864645	5.247891	0.562016
9	6	0	-1.600348	1.883225	-2.203400
10	6	0	-0.470631	3.127262	-0.577887
11	6	0	-2.210859	3.014824	-2.732466
12	1	0	-1.797335	0.901377	-2.621707
13	6	0	-1.064847	4.302019	-1.052481
14	6	0	-1.958015	4.285394	-2.152164
15	1	0	-2.880168	2.902786	-3.577136
16	1	0	-0.864645	5.247891	-0.562016
17	6	0	2.431095	0.444330	-2.203400
18	6	0	2.943604	-1.156052	-0.577887
19	6	0	3.716344	0.407248	-2.732466

20	1	0	1.679283	1.105850	-2.621707
21	6	0	4.258081	-1.228826	-1.052481
22	6	0	4.690268	-0.447007	-2.152164
23	1	0	3.953971	1.042906	-3.577136
24	1	0	4.977130	-1.875141	-0.562016
25	6	0	2.472973	-1.971209	0.577887
26	6	0	0.830747	-2.327555	2.203400
27	6	0	3.193235	-3.073194	1.052481
28	6	0	1.505485	-3.422072	2.732466
29	1	0	-0.118052	-2.007227	2.621707
30	6	0	2.732253	-3.838388	2.152164
31	1	0	4.112485	-3.372750	0.562016
32	1	0	1.073803	-3.945692	3.577136
33	6	0	-0.830747	-2.327555	-2.203400
34	6	0	-2.472973	-1.971209	-0.577887
35	6	0	-1.505485	-3.422072	-2.732466
36	1	0	0.118052	-2.007227	-2.621707
37	6	0	-3.193235	-3.073194	-1.052481
38	6	0	-2.732253	-3.838388	-2.152164
39	1	0	-1.073803	-3.945692	-3.577136
40	1	0	-4.112485	-3.372750	-0.562016
41	6	0	-2.943604	-1.156052	0.577887
42	6	0	-2.431095	0.444330	2.203400
43	6	0	-4.258081	-1.228826	1.052481
44	6	0	-3.716344	0.407248	2.732466
45	1	0	-1.679283	1.105850	2.621707
46	6	0	-4.690268	-0.447007	2.152164
47	1	0	-4.977130	-1.875141	0.562016
48	1	0	-3.953971	1.042906	3.577136
49	7	0	0.743418	1.919025	1.151202
50	7	0	-2.033633	-0.315694	1.151202
51	7	0	-1.290216	-1.603331	-1.151202
52	7	0	1.290216	-1.603331	1.151202
53	7	0	2.033633	-0.315694	-1.151202
54	7	0	-0.743418	1.919025	-1.151202
55	48	0	0.000000	0.000000	0.000000
56	6	0	-6.067503	-0.546810	2.600861
57	6	0	-6.629409	0.172028	3.615776
58	1	0	-6.693315	-1.252123	2.057049
59	1	0	-6.023680	0.902281	4.153200
60	6	0	-3.507303	-4.981207	-2.600861
61	6	0	-3.165724	-5.827250	-3.615776
62	1	0	-4.431028	-5.170520	-2.057049
63	1	0	-2.230442	-5.667800	-4.153200
64	6	0	6.067503	-0.546810	-2.600861
65	6	0	6.629409	0.172028	-3.615776
66	1	0	6.693315	-1.252123	-2.057049
67	1	0	6.023680	0.902281	-4.153200
68	6	0	3.507303	-4.981207	2.600861
69	6	0	3.165724	-5.827250	3.615776
70	1	0	4.431028	-5.170520	2.057049
71	1	0	2.230442	-5.667800	4.153200
72	6	0	2.560200	5.528017	2.600861
73	6	0	3.463685	5.655222	3.615776
74	1	0	2.262288	6.422642	2.057049
75	1	0	3.793238	4.765519	4.153200
76	6	0	-2.560200	5.528017	-2.600861
77	6	0	-3.463685	5.655222	-3.615776
78	1	0	-2.262288	6.422642	-2.057049
79	1	0	-3.793238	4.765519	-4.153200
80	6	0	3.926452	-6.975400	4.048452
81	6	0	5.272870	-7.358625	3.664190
82	6	0	3.466065	-7.948784	5.024521
83	6	0	5.610747	-8.561060	4.366377
84	1	0	2.497742	-7.947710	5.503801
85	6	0	4.496636	-8.926279	5.203223
86	1	0	6.546071	-9.095076	4.292395
87	1	0	4.451589	-9.782521	5.858861

88	1	0	5.911464	-6.839229	2.965446
89	6	0	8.004099	0.087293	-4.048452
90	6	0	9.009191	-0.887127	-3.664190
91	6	0	8.616881	0.972692	-5.024521
92	6	0	10.219469	-0.578519	-4.366377
93	1	0	8.131789	1.810747	-5.503801
94	6	0	9.978702	0.568939	-5.203223
95	1	0	11.149602	-1.121526	-4.292395
96	1	0	10.697706	1.036071	-5.858861
97	1	0	8.878678	-1.699864	-2.965446
98	6	0	4.077648	6.888107	4.048452
99	6	0	3.736321	8.245752	3.664190
100	6	0	5.150816	6.976092	5.024521
101	6	0	4.608722	9.139579	4.366377
102	1	0	5.634047	6.136963	5.503801
103	6	0	5.482066	8.357340	5.203223
104	1	0	4.603531	10.216602	4.292395
105	1	0	6.246117	8.746450	5.858861
106	6	0	-4.077648	6.888107	-4.048452
107	6	0	-3.736321	8.245752	-3.664190
108	6	0	-5.150816	6.976092	-5.024521
109	6	0	-4.608722	9.139579	-4.366377
110	1	0	-5.634047	6.136963	-5.503801
111	6	0	-5.482066	8.357340	-5.203223
112	1	0	-4.603531	10.216602	-4.292395
113	1	0	-6.246117	8.746450	-5.858861
114	1	0	-2.967214	8.539092	-2.965446
115	1	0	2.967214	8.539092	2.965446
116	6	0	-8.004099	0.087293	4.048452
117	6	0	-9.009191	-0.887127	3.664190
118	6	0	-8.616881	0.972692	5.024521
119	6	0	-10.219469	-0.578519	4.366377
120	1	0	-8.131789	1.810747	5.503801
121	6	0	-9.978702	0.568939	5.203223
122	1	0	-11.149602	-1.121526	4.292395
123	1	0	-10.697706	1.036071	5.858861
124	6	0	-3.926452	-6.975400	-4.048452
125	6	0	-5.272870	-7.358625	-3.664190
126	6	0	-3.466065	-7.948784	-5.024521
127	6	0	-5.610747	-8.561060	-4.366377
128	1	0	-2.497742	-7.947710	-5.503801
129	6	0	-4.496636	-8.926279	-5.203223
130	1	0	-6.546071	-9.095076	-4.292395
131	1	0	-4.451589	-9.782521	-5.858861
132	1	0	-5.911464	-6.839229	-2.965446
133	1	0	-8.878678	-1.699864	2.965446
134	26	0	-5.184935	-7.011861	-5.713527
135	26	0	-8.664917	-0.984355	5.713527
136	26	0	3.479982	7.996216	5.713527
137	26	0	-3.479982	7.996216	-5.713527
138	26	0	8.664917	-0.984355	-5.713527
139	26	0	5.184935	-7.011861	5.713527
140	6	0	-5.237625	-5.129834	-6.628885
141	1	0	-4.685202	-4.261305	-6.301072
142	6	0	-4.775890	-6.124486	-7.561888
143	6	0	-6.554553	-5.506756	-6.188280
144	1	0	-3.824429	-6.127295	-8.072357
145	6	0	-5.812255	-7.113100	-7.703320
146	1	0	-7.170827	-4.965331	-5.486230
147	6	0	-6.910324	-6.732710	-6.854831
148	1	0	-5.769388	-7.993013	-8.327511
149	1	0	-7.834357	-7.277731	-6.732874
150	6	0	-7.061379	-1.970999	6.628885
151	1	0	-6.032999	-1.926851	6.301072
152	6	0	-7.691905	-1.073799	7.561888
153	6	0	-8.046267	-2.923032	6.188280
154	1	0	-7.218608	-0.248405	8.072357
155	6	0	-9.066253	-1.477010	7.703320

156	1	0	-7.885516	-3.727453	5.486230
157	6	0	-9.285860	-2.618162	6.854831
158	1	0	-9.806846	-0.999930	8.327511
159	1	0	-10.219879	-3.145887	6.732874
160	6	0	5.237625	-5.129834	6.628885
161	1	0	4.685202	-4.261305	6.301072
162	6	0	4.775890	-6.124486	7.561888
163	6	0	6.554553	-5.506756	6.188280
164	1	0	3.824429	-6.127295	8.072357
165	6	0	5.812255	-7.113100	7.703320
166	1	0	7.170827	-4.965331	5.486230
167	6	0	6.910324	-6.732710	6.854831
168	1	0	5.769388	-7.993013	8.327511
169	1	0	7.834357	-7.277731	6.732874
170	6	0	1.823754	7.100833	6.628885
171	1	0	1.347798	6.188156	6.301072
172	6	0	2.916015	7.198285	7.561888
173	6	0	1.491714	8.429787	6.188280
174	1	0	3.394179	6.375701	8.072357
175	6	0	3.253998	8.590110	7.703320
176	1	0	0.714689	8.692784	5.486230
177	6	0	2.375535	9.350871	6.854831
178	1	0	4.037458	8.992943	8.327511
179	1	0	2.385522	10.423618	6.732874
180	6	0	-1.823754	7.100833	-6.628885
181	1	0	-1.347798	6.188156	-6.301072
182	6	0	-2.916015	7.198285	-7.561888
183	6	0	-1.491714	8.429787	-6.188280
184	1	0	-3.394179	6.375701	-8.072357
185	6	0	-3.253998	8.590110	-7.703320
186	1	0	-0.714689	8.692784	-5.486230
187	6	0	-2.375535	9.350871	-6.854831
188	1	0	-4.037458	8.992943	-8.327511
189	1	0	-2.385522	10.423618	-6.732874
190	6	0	7.061379	-1.970999	-6.628885
191	1	0	6.032999	-1.926851	-6.301072
192	6	0	7.691905	-1.073799	-7.561888
193	6	0	8.046267	-2.923032	-6.188280
194	1	0	7.218608	-0.248405	-8.072357
195	6	0	9.066253	-1.477010	-7.703320
196	1	0	7.885516	-3.727453	-5.486230
197	6	0	9.285860	-2.618162	-6.854831
198	1	0	9.806846	-0.999930	-8.327511
199	1	0	10.219879	-3.145887	-6.732874

E(RB3P86) = -5069.42223670 A.U.

Dication in 5:

Standard orientation:

Centre Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.557885	1.878944	2.229362
2	6	0	0.452242	3.131804	0.592827
3	6	0	2.130648	3.010991	2.796876
4	1	0	1.762347	0.893141	2.634594
5	6	0	1.007085	4.308723	1.109071
6	6	0	1.865268	4.288200	2.236491
7	1	0	2.777102	2.894396	3.658362
8	1	0	0.798879	5.261358	0.635503
9	6	0	-1.557885	1.878944	-2.229362
10	6	0	-0.452242	3.131804	-0.592827
11	6	0	-2.130648	3.010991	-2.796876

12	1	0	-1.762347	0.893141	-2.634594
13	6	0	-1.007085	4.308723	-1.109071
14	6	0	-1.865268	4.288200	-2.236491
15	1	0	-2.777102	2.894396	-3.658362
16	1	0	-0.798879	5.261358	-0.635503
17	6	0	2.406156	0.409696	-2.229362
18	6	0	2.938343	-1.174249	-0.592827
19	6	0	3.672919	0.339700	-2.796876
20	1	0	1.654656	1.079667	-2.634594
21	6	0	4.235006	-1.282200	-1.109071
22	6	0	4.646324	-0.528730	-2.236491
23	1	0	3.895171	0.957843	-3.658362
24	1	0	4.955909	-1.938829	-0.635503
25	6	0	2.486101	-1.957555	0.592827
26	6	0	0.848271	-2.288640	2.229362
27	6	0	3.227921	-3.026523	1.109071
28	6	0	1.542271	-3.350691	2.796876
29	1	0	-0.107691	-1.972808	2.634594
30	6	0	2.781056	-3.759470	2.236491
31	1	0	4.157030	-3.322529	0.635503
32	1	0	1.118069	-3.852239	3.658362
33	6	0	-0.848271	-2.288640	-2.229362
34	6	0	-2.486101	-1.957555	-0.592827
35	6	0	-1.542271	-3.350691	-2.796876
36	1	0	0.107691	-1.972808	-2.634594
37	6	0	-3.227921	-3.026523	-1.109071
38	6	0	-2.781056	-3.759470	-2.236491
39	1	0	-1.118069	-3.852239	-3.658362
40	1	0	-4.157030	-3.322529	-0.635503
41	6	0	-2.938343	-1.174249	0.592827
42	6	0	-2.406156	0.409696	2.229362
43	6	0	-4.235006	-1.282200	1.109071
44	6	0	-3.672919	0.339700	2.796876
45	1	0	-1.654656	1.079667	2.634594
46	6	0	-4.646324	-0.528730	2.236491
47	1	0	-4.955909	-1.938829	0.635503
48	1	0	-3.895171	0.957843	3.658362
49	7	0	0.730198	1.919211	1.154484
50	7	0	-2.027185	-0.327235	1.154484
51	7	0	-1.296986	-1.591976	-1.154484
52	7	0	1.296986	-1.591976	1.154484
53	7	0	2.027185	-0.327235	-1.154484
54	7	0	-0.730198	1.919211	-1.154484
55	6	0	-6.000928	-0.673891	2.739937
56	6	0	-6.528018	0.012764	3.796033
57	1	0	-6.623372	-1.392131	2.210060
58	1	0	-5.893876	0.735454	4.311010
59	6	0	-3.584071	-4.860011	-2.739937
60	6	0	-3.252955	-5.659812	-3.796033
61	1	0	-4.517307	-5.039943	-2.210060
62	1	0	-2.310016	-5.471973	-4.311010
63	6	0	6.000928	-0.673891	-2.739937
64	6	0	6.528018	0.012764	-3.796033
65	1	0	6.623372	-1.392131	-2.210060
66	1	0	5.893876	0.735454	-4.311010
67	6	0	3.584071	-4.860011	2.739937
68	6	0	3.252955	-5.659812	3.796033
69	1	0	4.517307	-5.039943	2.210060
70	1	0	2.310016	-5.471973	4.311010
71	6	0	2.416858	5.533901	2.739937
72	6	0	3.275063	5.647047	3.796033
73	1	0	2.106065	6.432074	2.210060
74	1	0	3.583860	4.736519	4.311010
75	6	0	-2.416858	5.533901	-2.739937
76	6	0	-3.275063	5.647047	-3.796033
77	1	0	-2.106065	6.432074	-2.210060
78	1	0	-3.583860	4.736519	-4.311010
79	6	0	6.140973	-10.117157	6.062333

80	6	0	7.483507	-10.552226	5.729317
81	6	0	5.650623	-11.012045	7.093082
82	6	0	7.797710	-11.702083	6.525859
83	1	0	4.678939	-10.977853	7.562167
84	6	0	6.665509	-11.987017	7.366360
85	1	0	8.726284	-12.252126	6.503355
86	1	0	6.593050	-12.791035	8.082967
87	1	0	8.144177	-10.097846	5.006391
88	6	0	11.832201	-0.259660	-6.062333
89	6	0	12.880249	-1.204794	-5.729317
90	6	0	12.362022	0.612440	-7.093082
91	6	0	14.033156	-0.901973	-6.525859
92	1	0	11.846569	1.436847	-7.562167
93	6	0	13.713816	0.221009	-7.366360
94	1	0	14.973794	-1.431120	-6.503355
95	1	0	14.373886	0.685769	-8.082967
96	1	0	12.817080	-2.004141	-5.006391
97	6	0	5.691229	10.376817	6.062333
98	6	0	5.396743	11.757020	5.729317
99	6	0	6.711400	10.399605	7.093082
100	6	0	6.235447	12.604056	6.525859
101	1	0	7.167630	9.541006	7.562167
102	6	0	7.048307	11.766008	7.366360
103	1	0	6.247511	13.683246	6.503355
104	1	0	7.780837	12.105266	8.082967
105	6	0	-5.691229	10.376817	-6.062333
106	6	0	-5.396743	11.757020	-5.729317
107	6	0	-6.711400	10.399605	-7.093082
108	6	0	-6.235447	12.604056	-6.525859
109	1	0	-7.167630	9.541006	-7.562167
110	6	0	-7.048307	11.766008	-7.366360
111	1	0	-6.247511	13.683246	-6.503355
112	1	0	-7.780837	12.105266	-8.082967
113	1	0	-4.672903	12.101987	-5.006391
114	1	0	4.672903	12.101987	5.006391
115	6	0	-11.832201	-0.259660	6.062333
116	6	0	-12.880249	-1.204794	5.729317
117	6	0	-12.362022	0.612440	7.093082
118	6	0	-14.033156	-0.901973	6.525859
119	1	0	-11.846569	1.436847	7.562167
120	6	0	-13.713816	0.221009	7.366360
121	1	0	-14.973794	-1.431120	6.503355
122	1	0	-14.373886	0.685769	8.082967
123	6	0	-6.140973	-10.117157	-6.062333
124	6	0	-7.483507	-10.552226	-5.729317
125	6	0	-5.650623	-11.012045	-7.093082
126	6	0	-7.797710	-11.702083	-6.525859
127	1	0	-4.678939	-10.977853	-7.562167
128	6	0	-6.665509	-11.987017	-7.366360
129	1	0	-8.726284	-12.252126	-6.503355
130	1	0	-6.593050	-12.791035	-8.082967
131	1	0	-8.144177	-10.097846	-5.006391
132	1	0	-12.817080	-2.004141	5.006391
133	26	0	-7.373613	-10.054482	-7.745379
134	26	0	-12.394243	-1.358496	7.745379
135	26	0	5.020630	11.412977	7.745379
136	26	0	-5.020630	11.412977	-7.745379
137	26	0	12.394243	-1.358496	-7.745379
138	26	0	7.373613	-10.054482	7.745379
139	6	0	-7.405096	-8.104195	-8.497570
140	1	0	-6.855376	-7.272496	-8.081447
141	6	0	-6.926007	-9.016867	-9.502171
142	6	0	-8.732370	-8.513693	-8.119369
143	1	0	-5.961694	-8.981111	-9.986701
144	6	0	-7.959961	-9.988655	-9.748412
145	1	0	-9.361620	-8.032686	-7.385430
146	6	0	-9.075564	-9.677990	-8.894092
147	1	0	-7.904295	-10.812431	-10.444289

148	1	0	-10.002334	-10.229124	-8.837344
149	6	0	-10.720987	-2.360904	8.497570
150	1	0	-9.725854	-2.300682	8.081447
151	6	0	-11.271839	-1.489665	9.502171
152	6	0	-11.739259	-3.305608	8.119369
153	1	0	-10.758717	-0.672423	9.986701
154	6	0	-12.630409	-1.899201	9.748412
155	1	0	-11.637320	-4.091058	7.385430
156	6	0	-12.919167	-3.020674	8.894092
157	1	0	-13.315987	-1.439105	10.444289
158	1	0	-13.859848	-3.547714	8.837344
159	6	0	7.405096	-8.104195	8.497570
160	1	0	6.855376	-7.272496	8.081447
161	6	0	6.926007	-9.016867	9.502171
162	6	0	8.732370	-8.513693	8.119369
163	1	0	5.961694	-8.981111	9.986701
164	6	0	7.959961	-9.988655	9.748412
165	1	0	9.361620	-8.032686	7.385430
166	6	0	9.075564	-9.677990	8.894092
167	1	0	7.904295	-10.812431	10.444289
168	1	0	10.002334	-10.229124	8.837344
169	6	0	3.315890	10.465099	8.497570
170	1	0	2.870478	9.573178	8.081447
171	6	0	4.345832	10.506532	9.502171
172	6	0	3.006889	11.819301	8.119369
173	1	0	4.797023	9.653534	9.986701
174	6	0	4.670448	11.887856	9.748412
175	1	0	2.275700	12.123744	7.385430
176	6	0	3.843603	12.698664	8.894092
177	1	0	5.411692	12.251536	10.444289
178	1	0	3.857514	13.776837	8.837344
179	6	0	-3.315890	10.465099	-8.497570
180	1	0	-2.870478	9.573178	-8.081447
181	6	0	-4.345832	10.506532	-9.502171
182	6	0	-3.006889	11.819301	-8.119369
183	1	0	-4.797023	9.653534	-9.986701
184	6	0	-4.670448	11.887856	-9.748412
185	1	0	-2.275700	12.123744	-7.385430
186	6	0	-3.843603	12.698664	-8.894092
187	1	0	-5.411692	12.251536	-10.444289
188	1	0	-3.857514	13.776837	-8.837344
189	6	0	10.720987	-2.360904	-8.497570
190	1	0	9.725854	-2.300682	-8.081447
191	6	0	11.271839	-1.489665	-9.502171
192	6	0	11.739259	-3.305608	-8.119369
193	1	0	10.758717	-0.672423	-9.986701
194	6	0	12.630409	-1.899201	-9.748412
195	1	0	11.637320	-4.091058	-7.385430
196	6	0	12.919167	-3.020674	-8.894092
197	1	0	13.315987	-1.439105	-10.444289
198	1	0	13.859848	-3.547714	-8.837344
199	6	0	4.017819	-6.768847	4.336961
200	6	0	3.484567	-7.494748	5.429931
201	6	0	5.276975	-7.178631	3.831396
202	6	0	4.166992	-8.571411	5.990164
203	1	0	2.518737	-7.204800	5.838434
204	6	0	5.957728	-8.254461	4.391524
205	1	0	5.724489	-6.655139	2.991329
206	6	0	5.424698	-8.979146	5.487617
207	1	0	3.727419	-9.102024	6.828087
208	1	0	6.913905	-8.551448	3.973072
209	6	0	7.870903	-0.095110	-4.336961
210	6	0	8.855364	-0.980679	-3.831396
211	6	0	8.232926	0.729651	-5.429931
212	6	0	10.127437	-1.032313	-4.391524
213	1	0	8.625764	-1.629983	-2.991329
214	6	0	9.506556	0.676985	-5.990164
215	1	0	7.498908	1.421110	-5.838434

216	6	0	10.488518	-0.208353	-5.487617
217	1	0	10.862724	-1.711893	-3.973072
218	1	0	9.746293	1.322973	-6.828087
219	6	0	3.853084	6.863957	4.336961
220	6	0	4.748359	6.765097	5.429931
221	6	0	3.578390	8.159310	3.831396
222	6	0	5.339564	7.894426	5.990164
223	1	0	4.980171	5.783690	5.838434
224	6	0	4.169709	9.286774	4.391524
225	1	0	2.901275	8.285122	2.991329
226	6	0	5.063820	9.187499	5.487617
227	1	0	6.018875	7.779051	6.828087
228	1	0	3.948819	10.263341	3.973072
229	6	0	-3.853084	6.863957	-4.336961
230	6	0	-3.578390	8.159310	-3.831396
231	6	0	-4.748359	6.765097	-5.429931
232	6	0	-4.169709	9.286774	-4.391524
233	1	0	-2.901275	8.285122	-2.991329
234	6	0	-5.339564	7.894426	-5.990164
235	1	0	-4.980171	5.783690	-5.838434
236	6	0	-5.063820	9.187499	-5.487617
237	1	0	-3.948819	10.263341	-3.973072
238	1	0	-6.018875	7.779051	-6.828087
239	6	0	-7.870903	-0.095110	4.336961
240	6	0	-8.232926	0.729651	5.429931
241	6	0	-8.855364	-0.980679	3.831396
242	6	0	-9.506556	0.676985	5.990164
243	1	0	-7.498908	1.421110	5.838434
244	6	0	-10.127437	-1.032313	4.391524
245	1	0	-8.625764	-1.629983	2.991329
246	6	0	-10.488518	-0.208353	5.487617
247	1	0	-9.746293	1.322973	6.828087
248	1	0	-10.862724	-1.711893	3.973072
249	6	0	-4.017819	-6.768847	-4.336961
250	6	0	-5.276975	-7.178631	-3.831396
251	6	0	-3.484567	-7.494748	-5.429931
252	6	0	-5.957728	-8.254461	-4.391524
253	1	0	-5.724489	-6.655139	-2.991329
254	6	0	-4.166992	-8.571411	-5.990164
255	1	0	-2.518737	-7.204800	-5.838434
256	6	0	-5.424698	-8.979146	-5.487617
257	1	0	-6.913905	-8.551448	-3.973072
258	1	0	-3.727419	-9.102024	-6.828087
259	48	0	0.000000	0.000000	0.000000

E(RB3P86) = -6459.90301338 A.U.

Dication in 6:

Standard orientation:

Centre Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.540588	1.878782	2.241414
2	6	0	0.446186	3.132071	0.597376
3	6	0	2.101970	3.011243	2.818945
4	1	0	1.746638	0.892294	2.644247
5	6	0	0.990379	4.309534	1.123246
6	6	0	1.835355	4.289664	2.260897
7	1	0	2.742363	2.894470	3.684962
8	1	0	0.782333	5.263019	0.651356
9	6	0	-1.540588	1.878782	-2.241414
10	6	0	-0.446186	3.132071	-0.597376
11	6	0	-2.101970	3.011243	-2.818945

12	1	0	-1.746638	0.892294	-2.644247
13	6	0	-0.990379	4.309534	-1.123246
14	6	0	-1.835355	4.289664	-2.260897
15	1	0	-2.742363	2.894470	-3.684962
16	1	0	-0.782333	5.263019	-0.651356
17	6	0	2.397367	0.394797	-2.241414
18	6	0	2.935546	-1.179627	-0.597376
19	6	0	3.658798	0.314738	-2.818945
20	1	0	1.646068	1.066486	-2.644247
21	6	0	4.227355	-1.297074	-1.123246
22	6	0	4.632635	-0.555368	-2.260897
23	1	0	3.877866	0.927721	-3.684962
24	1	0	4.949075	-1.953989	-0.651356
25	6	0	2.489360	-1.952444	0.597376
26	6	0	0.856779	-2.273579	2.241414
27	6	0	3.236976	-3.012460	1.123246
28	6	0	1.556828	-3.325981	2.818945
29	1	0	-0.100570	-1.958780	2.644247
30	6	0	2.797280	-3.734296	2.260897
31	1	0	4.166742	-3.309030	0.651356
32	1	0	1.135503	-3.822191	3.684962
33	6	0	-0.856779	-2.273579	-2.241414
34	6	0	-2.489360	-1.952444	-0.597376
35	6	0	-1.556828	-3.325981	-2.818945
36	1	0	0.100570	-1.958780	-2.644247
37	6	0	-3.236976	-3.012460	-1.123246
38	6	0	-2.797280	-3.734296	-2.260897
39	1	0	-1.135503	-3.822191	-3.684962
40	1	0	-4.166742	-3.309030	-0.651356
41	6	0	-2.935546	-1.179627	0.597376
42	6	0	-2.397367	0.394797	2.241414
43	6	0	-4.227355	-1.297074	1.123246
44	6	0	-3.658798	0.314738	2.818945
45	1	0	-1.646068	1.066486	2.644247
46	6	0	-4.632635	-0.555368	2.260897
47	1	0	-4.949075	-1.953989	0.651356
48	1	0	-3.877866	0.927721	3.684962
49	7	0	0.723374	1.918777	1.158337
50	7	0	-2.023397	-0.332928	1.158337
51	7	0	-1.300023	-1.585849	-1.158337
52	7	0	1.300023	-1.585849	1.158337
53	7	0	2.023397	-0.332928	-1.158337
54	7	0	-0.723374	1.918777	-1.158337
55	6	0	-5.980562	-0.713290	2.775708
56	6	0	-6.493290	-0.060894	3.861383
57	1	0	-6.610103	-1.415958	2.233438
58	1	0	-5.849866	0.640607	4.393853
59	6	0	-3.608008	-4.822674	-2.775708
60	6	0	-3.299381	-5.592907	-3.861383
61	1	0	-4.531307	-5.016538	-2.233438
62	1	0	-2.370151	-5.386436	-4.393853
63	6	0	5.980562	-0.713290	-2.775708
64	6	0	6.493290	-0.060894	-3.861383
65	1	0	6.610103	-1.415958	-2.233438
66	1	0	5.849866	0.640607	-4.393853
67	6	0	3.608008	-4.822674	2.775708
68	6	0	3.299381	-5.592907	3.861383
69	1	0	4.531307	-5.016538	2.233438
70	1	0	2.370151	-5.386436	4.393853
71	6	0	2.372554	5.535964	2.775708
72	6	0	3.193909	5.653801	3.861383
73	1	0	2.078796	6.432496	2.233438
74	1	0	3.479715	4.745829	4.393853
75	6	0	-2.372554	5.535964	-2.775708
76	6	0	-3.193909	5.653801	-3.861383
77	1	0	-2.078796	6.432496	-2.233438
78	1	0	-3.479715	4.745829	-4.393853
79	6	0	6.739320	-11.811221	7.779445

80	6	0	8.102210	-12.185160	7.455245
81	6	0	6.285900	-12.713087	8.821508
82	6	0	8.460901	-13.315387	8.262548
83	1	0	5.308058	-12.697771	9.280930
84	6	0	7.339877	-13.642343	9.105422
85	1	0	9.412543	-13.825256	8.249650
86	1	0	7.302247	-14.443762	9.827496
87	1	0	8.741176	-11.702542	6.730773
88	6	0	13.598477	0.069188	-7.779445
89	6	0	14.603763	-0.924140	-7.455245
90	6	0	14.152806	0.912794	-8.821508
91	6	0	15.761914	-0.669662	-8.262548
92	1	0	13.650621	1.751972	-9.280930
93	6	0	15.484554	0.464652	-9.105422
94	1	0	16.679294	-1.238873	-8.249650
95	1	0	16.159788	0.897950	-9.827496
96	1	0	14.505287	-1.718809	-6.730773
97	6	0	6.859157	11.742033	7.779445
98	6	0	6.501553	13.109300	7.455245
99	6	0	7.866906	11.800293	8.821508
100	6	0	7.301013	13.985049	8.262548
101	1	0	8.342563	10.945799	9.280930
102	6	0	8.144677	13.177691	9.105422
103	1	0	7.266751	15.064129	8.249650
104	1	0	8.857541	13.545812	9.827496
105	6	0	-6.859157	11.742033	-7.779445
106	6	0	-6.501553	13.109300	-7.455245
107	6	0	-7.866906	11.800293	-8.821508
108	6	0	-7.301013	13.985049	-8.262548
109	1	0	-8.342563	10.945799	-9.280930
110	6	0	-8.144677	13.177691	-9.105422
111	1	0	-7.266751	15.064129	-8.249650
112	1	0	-8.857541	13.545812	-9.827496
113	1	0	-5.764111	13.421351	-6.730773
114	1	0	5.764111	13.421351	6.730773
115	6	0	-13.598477	0.069188	7.779445
116	6	0	-14.603763	-0.924140	7.455245
117	6	0	-14.152806	0.912794	8.821508
118	6	0	-15.761914	-0.669662	8.262548
119	1	0	-13.650621	1.751972	9.280930
120	6	0	-15.484554	0.464652	9.105422
121	1	0	-16.679294	-1.238873	8.249650
122	1	0	-16.159788	0.897950	9.827496
123	6	0	-6.739320	-11.811221	-7.779445
124	6	0	-8.102210	-12.185160	-7.455245
125	6	0	-6.285900	-12.713087	-8.821508
126	6	0	-8.460901	-13.315387	-8.262548
127	1	0	-5.308058	-12.697771	-9.280930
128	6	0	-7.339877	-13.642343	-9.105422
129	1	0	-9.412543	-13.825256	-8.249650
130	1	0	-7.302247	-14.443762	-9.827496
131	1	0	-8.741176	-11.702542	-6.730773
132	1	0	-14.505287	-1.718809	6.730773
133	26	0	-7.966553	-11.679647	-9.470064
134	26	0	-14.098148	-1.059414	9.470064
135	26	0	6.131595	12.739061	9.470064
136	26	0	-6.131595	12.739061	-9.470064
137	26	0	14.098148	-1.059414	-9.470064
138	26	0	7.966553	-11.679647	9.470064
139	6	0	-7.921414	-9.722609	-10.207958
140	1	0	-7.339455	-8.916170	-9.786315
141	6	0	-7.481447	-10.646720	-11.220709
142	6	0	-9.262223	-10.081672	-9.828414
143	1	0	-6.518009	-10.646082	-11.708372
144	6	0	-8.554273	-11.573522	-11.471816
145	1	0	-9.868436	-9.581770	-9.087824
146	6	0	-9.653992	-11.225635	-10.611047
147	1	0	-8.533255	-12.393693	-12.173893

148	1	0	-10.602358	-11.738943	-10.556157
149	6	0	-12.380733	-1.998841	10.207958
150	1	0	-11.391357	-1.898069	9.786315
151	6	0	-12.961053	-1.155763	11.220709
152	6	0	-13.362096	-2.980484	9.828414
153	1	0	-12.478782	-0.321720	11.708372
154	6	0	-14.300101	-1.621457	11.471816
155	1	0	-13.232274	-3.755431	9.087824
156	6	0	-14.548681	-2.747785	10.611047
157	1	0	-14.999880	-1.193169	12.173893
158	1	0	-15.467402	-3.312440	10.556157
159	6	0	7.921414	-9.722609	10.207958
160	1	0	7.339455	-8.916170	9.786315
161	6	0	7.481447	-10.646720	11.220709
162	6	0	9.262223	-10.081672	9.828414
163	1	0	6.518009	-10.646082	11.708372
164	6	0	8.554273	-11.573522	11.471816
165	1	0	9.868436	-9.581770	9.087824
166	6	0	9.653992	-11.225635	10.611047
167	1	0	8.533255	-12.393693	12.173893
168	1	0	10.602358	-11.738943	10.556157
169	6	0	4.459319	11.721450	10.207958
170	1	0	4.051902	10.814239	9.786315
171	6	0	5.479606	11.802483	11.220709
172	6	0	4.099873	13.062156	9.828414
173	1	0	5.960773	10.967802	11.708372
174	6	0	5.745828	13.194979	11.471816
175	1	0	3.363838	13.337201	9.087824
176	6	0	4.894689	13.973420	10.611047
177	1	0	6.466625	13.586862	12.173893
178	1	0	4.865044	15.051383	10.556157
179	6	0	-4.459319	11.721450	-10.207958
180	1	0	-4.051902	10.814239	-9.786315
181	6	0	-5.479606	11.802483	-11.220709
182	6	0	-4.099873	13.062156	-9.828414
183	1	0	-5.960773	10.967802	-11.708372
184	6	0	-5.745828	13.194979	-11.471816
185	1	0	-3.363838	13.337201	-9.087824
186	6	0	-4.894689	13.973420	-10.611047
187	1	0	-6.466625	13.586862	-12.173893
188	1	0	-4.865044	15.051383	-10.556157
189	6	0	12.380733	-1.998841	-10.207958
190	1	0	11.391357	-1.898069	-9.786315
191	6	0	12.961053	-1.155763	-11.220709
192	6	0	13.362096	-2.980484	-9.828414
193	1	0	12.478782	-0.321720	-11.708372
194	6	0	14.300101	-1.621457	-11.471816
195	1	0	13.232274	-3.755431	-9.087824
196	6	0	14.548681	-2.747785	-10.611047
197	1	0	14.999880	-1.193169	-12.173893
198	1	0	15.467402	-3.312440	-10.556157
199	6	0	4.075467	-6.685998	4.414875
200	6	0	3.578282	-7.366258	5.556241
201	6	0	5.314473	-7.122203	3.881281
202	6	0	4.272065	-8.421873	6.137660
203	1	0	2.629261	-7.051826	5.985727
204	6	0	6.007688	-8.177925	4.462314
205	1	0	5.736268	-6.633018	3.008039
206	6	0	5.511839	-8.860552	5.605453
207	1	0	3.851622	-8.912173	7.009696
208	1	0	6.954881	-8.496745	4.034479
209	6	0	7.827978	-0.186459	-4.414875
210	6	0	8.825245	-1.041367	-3.881281
211	6	0	8.168508	0.584246	-5.556241
212	6	0	10.086135	-1.113848	-4.462314
213	1	0	8.612496	-1.651245	-3.008039
214	6	0	9.429588	0.511220	-6.137660
215	1	0	7.421691	1.248906	-5.985727

216	6	0	10.429383	-0.343117	-5.605453
217	1	0	10.835838	-1.774731	-4.034479
218	1	0	9.643979	1.120484	-7.009696
219	6	0	3.752511	6.872457	4.414875
220	6	0	4.590226	6.782012	5.556241
221	6	0	3.510772	8.163570	3.881281
222	6	0	5.157523	7.910653	6.137660
223	1	0	4.792430	5.802920	5.985727
224	6	0	4.078447	9.291773	4.462314
225	1	0	2.876228	8.284263	3.008039
226	6	0	4.917544	9.203669	5.605453
227	1	0	5.792357	7.791689	7.009696
228	1	0	3.880957	10.271476	4.034479
229	6	0	-3.752511	6.872457	-4.414875
230	6	0	-3.510772	8.163570	-3.881281
231	6	0	-4.590226	6.782012	-5.556241
232	6	0	-4.078447	9.291773	-4.462314
233	1	0	-2.876228	8.284263	-3.008039
234	6	0	-5.157523	7.910653	-6.137660
235	1	0	-4.792430	5.802920	-5.985727
236	6	0	-4.917544	9.203669	-5.605453
237	1	0	-3.880957	10.271476	-4.034479
238	1	0	-5.792357	7.791689	-7.009696
239	6	0	-7.827978	-0.186459	4.414875
240	6	0	-8.168508	0.584246	5.556241
241	6	0	-8.825245	-1.041367	3.881281
242	6	0	-9.429588	0.511220	6.137660
243	1	0	-7.421691	1.248906	5.985727
244	6	0	-10.086135	-1.113848	4.462314
245	1	0	-8.612496	-1.651245	3.008039
246	6	0	-10.429383	-0.343117	5.605453
247	1	0	-9.643979	1.120484	7.009696
248	1	0	-10.835838	-1.774731	4.034479
249	6	0	-4.075467	-6.685998	-4.414875
250	6	0	-5.314473	-7.122203	-3.881281
251	6	0	-3.578282	-7.366258	-5.556241
252	6	0	-6.007688	-8.177925	-4.462314
253	1	0	-5.736268	-6.633018	-3.008039
254	6	0	-4.272065	-8.421873	-6.137660
255	1	0	-2.629261	-7.051826	-5.985727
256	6	0	-5.511839	-8.860552	-5.605453
257	1	0	-6.954881	-8.496745	-4.034479
258	1	0	-3.851622	-8.912173	-7.009696
259	6	0	6.289601	-9.959757	6.160275
260	6	0	5.954191	-10.720398	7.239663
261	1	0	7.222505	-10.181962	5.643711
262	1	0	5.014450	-10.530679	7.758266
263	6	0	-6.289601	-9.959757	-6.160275
264	6	0	-5.954191	-10.720398	-7.239663
265	1	0	-7.222505	-10.181962	-5.643711
266	1	0	-5.014450	-10.530679	-7.758266
267	6	0	-11.770203	-0.467076	6.160275
268	6	0	-12.261233	0.203718	7.239663
269	1	0	-12.429090	-1.163892	5.643711
270	1	0	-11.627061	0.922698	7.758266
271	6	0	-5.480602	10.426833	-6.160275
272	6	0	-6.307042	10.516680	-7.239663
273	1	0	-5.206585	11.345854	-5.643711
274	1	0	-6.612611	9.607981	-7.758266
275	6	0	5.480602	10.426833	6.160275
276	6	0	6.307042	10.516680	7.239663
277	1	0	5.206585	11.345854	5.643711
278	1	0	6.612611	9.607981	7.758266
279	6	0	11.770203	-0.467076	-6.160275
280	6	0	12.261233	0.203718	-7.239663
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